

# The statistical description of irregular eigenfunctions: A semiclassical approach



## Dissertation

zur Erlangung des Doktorgrades  
der Naturwissenschaften (Dr. rer. nat.)  
der Naturwissenschaftlichen Fakultät II – Physik  
der Universität Regensburg

vorgelegt von

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July 2004

Die Arbeit wurde von Prof. Dr. Klaus Richter angeleitet.  
Das Promotionsgesuch wurde am 7. Juli 2004 eingereicht.  
Das Promotionskolloquium fand am 27. Juli 2004 statt.

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A Katalin, por permitirme tomar su mano, y por tomar la mia

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# Chapter 1

## Introduction

### 1.1 The time-spatial approach to quantum mechanics

Quantum mechanics is, as far as we know, the correct description of physical phenomena in the microscopic domain, and modern experimental techniques allow us to extend its predictions into the so-called mesoscopic regime, where manifestations of quantum coherence can be observed even on macroscopic scales.

By the end of the thirties two formulations of quantum mechanics were already known [1]. On one side the wave mechanics, based on a space of square integrable functions, the Schrödinger equation as dynamical law, and the Born rule to interpret the wavefunction as a probability amplitude. On the other side the matrix mechanics, based on a linear space with a dynamical law given by the Heisenberg equations and the physical observables represented by matrices. The works of Schrödinger, Von Newmman and Dirac finally brought a unified frame, the representation theory, in which both the wave and matrix pictures appear naturally as different representations of the same abstract theory [2].

In its final form by the thirties non-relativistic quantum mechanics then consisted of a Hilbert space with observables defined as linear operators acting on it, and a dynamical law given by the Schrödinger equation

$$\hat{H}|\psi(t)\rangle = -i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle, \quad (1.1)$$

where  $\hat{H}$  is the Hamilton operator. The physical content of the theory comes by taking the vectors in Hilbert space as physical states and postulating the inner product  $\langle a|\psi(t)\rangle$  as the probability amplitude to find the system in the state  $|a\rangle$  at time  $t$  (Born's rule).

Following a suggestion made by Dirac [3], Feynman re-introduced a pure time-space formulation of quantum mechanics in his classic 1948 paper [4]. Feynman approach is, in a sense, much more operational than the Hilbert space one in that it deals directly with the propagator, defined as the probability amplitude to find the system at the position  $\vec{r}_f$  at time  $t_f$  if it was at the position  $\vec{r}_i$  at time  $t_i$ . The Feynman propagator is formally given by

$$K(\vec{r}_i, t_i; \vec{r}_f, t_f) = \int e^{\frac{i}{\hbar} R[q(t)]} D[q(t)] \quad (1.2)$$

where the integral extends over the infinite dimensional space of continuous paths joining point  $\vec{r}_i$  at time  $t_i$  with point  $\vec{r}_f$  at time  $t_f$ .  $R[q(t)]$  is the action integral given by the line integral of the Lagrangian along the path  $q(t)$

$$R[q(t)] = \int_{q(t)} L(q(t), \dot{q}(t), t) dt. \quad (1.3)$$

The connection with the Schrödinger picture comes from the identity, valid for any conservative system with time-reversal symmetry (real eigenfunctions) [2]:

$$K(\vec{r}_i, t_i; \vec{r}_f, t_f) = \sum_{n=1}^{\infty} e^{-\frac{i}{\hbar}(E_n - i0^+)(t_f - t_i)} \psi_n(\vec{r}_i) \psi_n(\vec{r}_f), \quad (1.4)$$

where  $\psi_1(\vec{r}_i), \psi_2(\vec{r}_i), \dots$  are the eigenstates of the Hamilton operator in position representation and  $E_1, E_2, \dots$  the corresponding eigenvalues, which are discrete in the case of bounded systems that concern us here.

Often, a more useful object is the Fourier transform of  $K(\vec{r}_i, t_i; \vec{r}_f, t_f)$  to the energy domain, the Green function, given in terms of the eigenfunctions and eigenenergies as [2]

$$G(\vec{r}_i, \vec{r}_f, z) = \sum_{n=1}^{\infty} \frac{\psi_n(\vec{r}_i) \psi_n(\vec{r}_f)}{z - E_n}, \quad (1.5)$$

since it provides an operational definition of the spectrum and eigenfunctions of a given conservative bounded system: *the Green function is a meromorphic*



*function of the complex energy with poles at, and only at, the real eigenenergies and the wavefunctions given by the corresponding residues.*

We remark that even though it seems that the Feynman formulation is strongly dependent on the position representation, it provides a consistent and independent version of the theory. The fact that we can use time-space concepts in order to explore even pure spectral (representation independent) quantities will turn out to be a strong advantage of this approach.

Another advantage of the path integral approach is that it provides the starting point to construct a non-perturbative approximation scheme in which only classical information is used to construct the propagator: the *semiclassical approximation*.

## 1.2 Modern semiclassical techniques

There are few systems where the quantum mechanical equations can be exactly solved and the spectrum and eigenfunctions explicitly calculated. In fact, there is a whole branch of the mathematical physics dedicated to extend our knowledge about the class of exactly solvable systems [5]. Methods of approximation are required and have been available since the birth of quantum mechanics.

Following Berry and Mount [6], we classify the methods of approximation in quantum mechanics into three broad types:

- *perturbation theory*, where the quantities of interest are expressed as an infinite (and often divergent) expansion in some small parameter,
- *variational methods*, where the best approximate solution is selected out from a given set of trial functions, and
- *semiclassical techniques*, where the quantum mechanical quantities are expressed as asymptotic series in the (effective) Planck's constant.

The domain of validity of the semiclassical methods is bounded by the domain of validity of the stationary phase approximation involved in the derivation of the semiclassical approximation to the propagator [7]. Without going into details, usually such domain is given by the condition

$$\frac{\hbar}{S_{cl}} = \hbar_{eff} \ll 1 \tag{1.6}$$

where  $S_{cl}$  is an  $\hbar$ -independent characteristic classical action (a rough estimate for  $S_{cl}$  is  $\langle p \rangle L$  with  $\langle p \rangle$  the average momenta for given energy and  $L$  the linear system size). Except for pathological examples, this condition is achieved in the regime of high energies and/or high quantum numbers, a domain that we will refer to in the following as the *semiclassical regime*.

At this point a comment about semantics is in order. Even when the early attempts to construct a theory of atomic spectra were rooted into classical mechanics (Bohr's quantization rules), the first use of the classical dynamics as an approximation to the real quantum evolution in the framework of the modern theory was formalized by Ehrenfest [1]. The Ehrenfest theorem can be summarized by stating that for a wave packet the equations of motion of the expectation values of position and momenta are given by the classical equations of Hamilton. Pictorially, such quantum-classical correspondence breaks down at the time quantum fluctuations around the average behavior are large enough to produce interference among different parts of the wave packet (the so-called Ehrenfest time). Modern semiclassical techniques are, however, based on a representation of the quantum propagator which takes into account interference effects, and this approximation goes far beyond the limitations of the simple quantum-classical correspondence encoded in the Ehrenfest theorem.

Sadly, this misconception about semiclassical techniques, considering them more as a naive use of classical mechanics rather than as a full quantum mechanical scheme, has been taken as granted for years and even in very respectful textbooks [8]. *All along this work we will stress the fact that semiclassical methods provide a consistent scheme to calculate quantum mechanical quantities by means of classical information only, but incorporating interference effects.*

In order to stress this point we can consider the following question. Since the semiclassical regime is defined by the existence of a small parameter, namely the effective Planck's constant  $\hbar_{eff}$ , are then the semiclassical expressions perturbative in  $\hbar_{eff}$ ? The answer is no. The reason is that, as can be easily seen, the dependence on  $\hbar_{eff}$  in the quantum propagator is non analytical. In fact, the value  $\hbar_{eff} = 0$  is an essential singularity and then its vicinity can not be studied using any kind of finite-order perturbative treatment. The power of the semiclassical approximation lies in the fact that such a singular behavior, the one being responsible for the interference effects, is respected when the main approximation tool, the stationary phase approximation, is used. After the singularity is properly taken into account,

what is left can be treated with standard perturbative techniques.

After this short turn into semantics, we come back now to the formalism of the semiclassical methods. Historically, the first attempt to deal with the singular character of the  $\hbar_{eff} \rightarrow 0$  limit was proposed by Wentzel, Kramers and Brillouin for one-dimensional problems and is the well known WKB approximation [1]. Shortly after, Van Vleck tried to generalize the method to deal with multi-dimensional systems where the Schrödinger equation is non-separable (the separable case is formally identical to a collection of one-dimensional problems). The so-called Van Vleck propagator faced two problems [7]. First, it is divergent at the points where the classical trajectories have turning points, making it valid only for extremely short times. This alone was not a reason to make the approach useless, since one can always consider the propagator far away from the turning points, as it was already in use within the WKB method. The second problem was that there was no known way to connect the different solutions corresponding to classical paths before and after the turning points. This is the so-called connection problem and it was responsible for putting the Van Vleck propagator into oblivion for years.

This was the state of the affair when in a series of classic papers, Gutzwiller [9] successfully applied the method of stationary phase approximation to the Feynman propagator. The divergences at the turning points were still there, but the connection problem was solved by using an extension of classical mechanics dealing with the behavior of non-classical paths around the classical ones. Morse theory [7] finally gives the recipes to add suitable phases to the semiclassical expressions and connect correctly the regions before and after the divergences.

The result of this analysis is the semiclassical approximation to the propagator, or simply *semiclassical propagator* given as a sum over classical paths,

$$K^{sc}(\vec{r}_i, t_i; \vec{r}_f, t_f) = \sum_p A_p(\vec{r}_i, t_i; \vec{r}_f, t_f) e^{\frac{i}{\hbar} R_p(\vec{r}_i, t_i; \vec{r}_f, t_f) + i\nu_p \frac{\pi}{4}}. \quad (1.7)$$

After a Fourier transform to the energy domain one obtains the most important result of the semiclassical analysis, the semiclassical (Gutzwiller) Green function [10]:

$$G^{sc}(\vec{r}_i, \vec{r}_f, e) = \sum_p \sqrt{|D_p(\vec{r}_i, t_i, e)|} e^{\frac{i}{\hbar} S_p(\vec{r}_i, \vec{r}_f, e) + i\nu_p \frac{\pi}{4}}, \quad (1.8)$$

where the sum runs over all classical paths  $p$  joining  $\vec{r}_i$  and  $\vec{r}_f$  at given energy  $e$ ,  $S_p(\vec{r}_i, \vec{r}_f, e) = \int_p \vec{p} \cdot d\vec{r}$  is the corresponding action,  $D_p(\vec{r}_i, t_i, e)$  an amplitude depending on the stability properties of the trajectory, and  $\nu_p$  is a topological index that solves the connection problem.

It is impossible to overestimate the importance of this expression and the huge amount of understanding and developments it has produced. In the semiclassical regime, all information about the quantum system can be recovered using this sum, including interference effects, in terms of pure classical information encoded in the action and stability properties of the classical trajectories.

### 1.3 The semiclassical approximation to the energy spectrum: Integrable vs. chaotic classical dynamics

Once the semiclassical Green function is derived, the location of its poles will tell us the location of the (semiclassical approximation to the) energy levels. Such calculation must be done, however, with extreme caution, because the meromorphic structure of the Green function is partially lost during the manipulations leading to its semiclassical approximation [11]. Very sophisticated methods of analytical continuation [20] must be used, and one ends with an equation of the form

$$\det(1 - \mathbf{T}(E)) = 0, \quad (1.9)$$

which in semiclassical approximation is a polynomial equation, with zeros at the semiclassical approximations to the energy levels. The particular form of the operator  $\mathbf{T}(E)$  depends on the method used, and in the future it will be referred to as the Bogomolny's transfer operator [13]. In any case it can be explicitly constructed using only classical information. Unitarity of the quantum evolution as well as independence on the representation are easily proven [13].

Even when for practical purposes the Eq. (1.9) is the most efficient method to locate the semiclassical approximation to the eigenenergies, there are many situations where the spectral density of states, defined as

$$\rho(E) = \sum_n \delta(E - E_n), \quad (1.10)$$

is required. This function can be explicitly constructed through the spectral determinant  $z(E) = \det(1 - \mathbf{T}(E))$ . Using the relationship between determinants and traces and performing an asymptotic expansion, one finds an expression for the density of states as a sum over the classical periodic orbits of the system

$$\rho(E) = \sum_p A_p(E) e^{\frac{i}{\hbar} S_p(E)}. \quad (1.11)$$

When written explicitly in terms of the structures in the classical phase space, this formula looks different depending on whether the classical dynamics is

- *chaotic* (all the classical periodic orbits are isolated) or
- *integrable* (all the classical periodic orbits come in continuous families).

In the chaotic case this formula is known as Gutzwiller trace formula [7], while in the integrable case it is known as Berry-Tabor trace formula [14]. These fundamental results are widely used to study quantum effects in the semiclassical regime in atomic [15], mesoscopic [16], molecular physics [17] and field theory [18].

## 1.4 The semiclassical theory of eigenfunctions

The quantum eigenstates of a system are given by the residues of the Green function at the eigenenergies. In principle, therefore, we should be able to derive a semiclassical expression for the wave functions, once we have the Green function. There is, however, a problem with this program: the semiclassical approximation to the Green function is no longer meromorphic. This means that, in the framework of Gutzwiller's theory, the semiclassical expression for the wave functions requires special care.

Before the Gutzwiller Green function appeared, another very powerful method to construct eigenfunctions in classically integrable systems was proposed by Keller and Maslov, the *torus quantization* [14], while a very sophisticated resummation technique was recently put forward by Prange, Fishmann and Georgeot in order to construct semiclassical approximations to the quantum eigenstates for both classically chaotic and integrable systems by means of the *Fredholm theory* of integral equations [11]. We briefly discuss this alternative approaches now.

### 1.4.1 Integrable case: Torus quantization

Classical integrable systems are characterized by the existence of classical invariant manifolds [19]. The importance of such structures for the semiclassical program was already remarked by Einstein in his attempts to derive a canonically invariant form of Bohr's quantization rules [14]. This program was finally developed as a formidable mathematical apparatus by Maslov and Keller, and it is since then known as "Torus quantization". The application of Fredholm's technique for such systems gives the same results, so we stick to a more physical presentation.

A classical integrable system with  $d$  degrees of freedom is characterized by the existence of  $d$  smooth (probably multi-valued) functions of the positions and momenta which are independent constants of motion [19]. A fundamental result of classical mechanics, the Poisson-Arnold theorem, states that the phase space is foliated by smooth manifolds with the topology of  $d$ -tori.

Given the set of constants of motion, it is always possible to perform a canonical transformation to a new set of phase-space coordinates, called action-angle variables, such that the coordinates (angles) evolve linearly in time while the momenta (actions) are constant. The set of angle coordinates define then a point on the torus, and its dimensions are given by the values of the action constants.

Semiclassical quantization comes by assigning quantum wave functions to each torus satisfying the Einstein-Brillouin-Keller conditions which relate the value of the actions with integer multiples of Planck's constant. The subset of tori with those particular actions are called "quantized tori" and the corresponding states are called "quasi-modes".

The quantum states constructed in this way are defined on phase space, and in order to have a wave function in configuration (or momentum) space one needs to project the torus. This projection will typically have singularities [20] and will assign many phase space points to a given position. The superposition principle is then invoked to add up the contributions from the different branches, and appropriate phases must be included in order to deal with the connection problem. Single-valuedness of the wavefunction on the torus gives rise to the selection of the quantized tori, which define then the semiclassical approximation to the eigenstates and eigenenergies of the quantum system (the latter are given by the value of the classical Hamiltonian on the torus).

### 1.4.2 Chaotic case: The Fredholm technique

As already pointed out by Einstein [21], non-integrable systems, where the number of degrees of freedom exceeds the number of independent constants of motion, can not be treated by torus quantization. At the beginning of the XX century the existence of such chaotic systems was recognized only by a small community in the area of mathematical physics, and the particular problems they pose were not recognized due to the belief that any quantum system could be treated by a combination of the integrable techniques and perturbation theory.

This issue was revived in 1970 by Percival [22] who conjectured that in the semiclassical limit, the spatial structure of eigenfunctions could be used to unambiguously classify them as *regular* eigenstates, corresponding to quantized tori, and *irregular* eigenstates corresponding to regions of classically chaotic behavior. Contrary to the integrable eigenfunctions, it took more than 30 years to provide a consistent semiclassical theory of irregular eigenfunctions in the form of the residues at the poles of the Fredholm Green function.

The Fredholm Green function applies a particular resummation technique in order to recover the meromorphic structure of the semiclassical Green function, lost during the application of the stationary phase approximation to the Feynmann propagator. Once we have a meromorphic Green function again, the semiclassical approximation to the eigenfunctions is unambiguously identified as the residues at the poles, the latter being the semiclassical approximation to the eigenenergies. The results of Fredholm theory are identical to the torus quantization method in the case of classically integrable dynamics, but they provide also results for the much more demanding case of classically chaotic dynamics.

Although the Fredholm residues are the best that semiclassical methods can do about eigenfunctions in classically chaotic systems, their practical calculation faces a delicate technical problem: the resulting expression requires a huge amount of classical information, namely, the knowledge of periodic orbits, its actions and stabilities up to a period given by the Heisenberg time, an extremely large time scale in classical terms that scales as  $\hbar_{eff}^{-1}$ .

There is also a more deep, conceptual problem with the use of the Fredholm theory of eigenfunctions: even when one could provide all the classical information required by the theory, it is known since many years that much of this highly system-specific information is washed out after averaging

mechanisms which are typically present in the experimental situations. The resulting statistical averages show an impressive degree of universality, in the sense that their main features can be very well explained by using theories with very few or no system-dependent parameters.

So far, the emergence of such universality is one of the open and fundamental questions in our understanding of the quantum-classical correspondence. Presently, however, we have no idea how to use the Fredholm residues to achieve a better understanding of the statistical properties of eigenfunctions in classically chaotic systems.

## **1.5 The statistical description of classically chaotic quantum systems: What is this thesis about?**

On the classical side, chaotic systems present a remarkable property: they can be characterized by means of statistical methods, and its statistical properties present a high degree of universality.

The use of statistical techniques when dealing with chaotic systems in classical mechanics is very old, and was strongly motivated by the discovery of the microscopic (Hamiltonian) foundations of classical statistical physics by Boltzmann, Gibbs and Maxwell and the qualitative study of phase space in chaotic systems initiated by Poincaré. For an excellent book on the subject see [23].

On the quantum side statistical methods are also useful. An example is the study of systems where the output (either experimental or theoretical) consist in such a huge amount of data that a level-by-level or eigenfunction-by-eigenfunction approach has no much sense.

The statistical study of quantum spectra rapidly became a subject on its own [24]. In particular the relationship between classically chaotic behavior and universal quantum spectral fluctuations described by the Random Matrix Theory [25] has been an intensive area of research for almost 20 years [26]. Presently we can say that Gutzwiller's theory provides a way for understanding of both universal and non-universal statistical properties of quantum spectra in classically chaotic systems.

The situation concerning the statistical properties of eigenfunctions in classically chaotic systems is, on the contrary, far from being well under-



stood. There are reasons for this. A very serious (and pure technical) one is that the main object of a statistical theory of eigenfunctions is the corresponding probability distribution, but this object is defined in the space of functions. We are dealing with a *functional* distribution, with all the well known problems of regularisation and convergence together with the far more difficult structure of the involved expressions (as compared to finite-dimensional spaces).

Lacking a microscopic ground for the statistical description of eigenfunctions, different methods based on different assumptions have been implemented so far, the two most popular being the Random Wave Models (assuming the wavefunction to be a random superposition of some basis functions) and the ballistic version of the Nonlinear Sigma Model (the theory of wavefunctions in disordered media). Both approaches have their strengths and limitations, and in some sense they can be seen as complementary.

In this work we present a third method to statistically describe eigenfunctions in closed and clean (i.e. disorder-free) quantum systems with chaotic classical counterpart. Our approach is semiclassical in spirit and has its roots in an observation made by Berry [27] already 30 years ago: eigenfunctions of classically chaotic quantum systems can be well described by random Gaussian fields.

The so-called Gaussian conjecture was modified and extended since then, but its definite and fully consistent form was presented only few years ago. A great advantage of the approach based on the Gaussian conjecture is, as we will show later, that it relies on an averaged version of the semiclassical Green function, and its main features (but not all!) can be incorporated by means of the Gutzwiller Green function, an object very tractable and far easier to manipulate than its Fredholm counterpart

Our goal in this work is to present and discuss the Gaussian conjecture and the semiclassical approximation to the two-point correlation function, the two only ingredients of our approach, and connect the resulting theory with the old versions and recent developments of the Random Wave Models, the Random Matrix Theory and the Nonlinear Sigma Model, together with specific applications and predictions of the theory beyond the scope of other approaches. The structure of this thesis is as follows:

In chapter II, after introducing an illustrative example of the use of statistical ideas when dealing with eigenfunctions in classically chaotic quantum systems, we provide the definition and carefully explain the main features of the different kinds of averaging mechanisms (spatial, spectral and over

disorder). Then we introduce and explain the different existing theories to describe statistically the eigenfunctions (the isotropic and non-isotropic Random Wave Models with their extensions, and the diffusive Nonlinear Sigma Model with its conjectured ballistic extension). To illustrate the different approaches we explicitly show their predictions for some relevant statistical measures. We focus on the emergence of the universal properties, in particular the celebrated universal result of Berry [27].

We formally introduce the spatial two-point correlation function in chapter III. After providing the formal correspondence with the Green function, we study the resulting semiclassical approximation to the correlation function, showing in which regimes the universal result of Berry is expected to hold. We present some important scaling relationships between the universal and system specific contributions and present a very demanding numerical check of our results for a specific (but generic) chaotic system. Finally, we mention the limitations of the approach based on the Gutzwiller Green function.

Chapter IV will be dedicated to present and carefully discuss the second ingredient of our approach, namely the Gaussian conjecture. After introducing the conjecture in an strict mathematical way, we critically review the existing arguments to support it (from semiclassics, information theory and quantum ergodicity), as well as its more evident drawback (the normalization problem). We perform also a very demanding numerical check of the conjecture for a generic chaotic system, and briefly discuss related numerical and experimental evidence supporting it.

Putting the pieces together, we present the full structure of our approach in chapter V. After introducing the main mathematical tool (Wick's theorem), we explicitly use the scaling of the different terms in the semiclassical two-point correlation function to drastically simplify the results of the theory. This provides a consistent semiclassical expansion of any average calculated within our approach. Finally, another fundamental concept is presented (Berry's diagonal approximation), which allows us to consistently split our results into non-oscillatory and oscillatory contributions.

Chapters VI and VII are entirely dedicated to applications of our ideas. In chapter VI we explore pure formal consequences of the theory. First, we show how to derive the results of the Random Wave Models as certain well controlled limits of our more general approach. After that, we formally establish the correspondence of the ballistic version of the Nonlinear Sigma Model with a highly pathological limit of the diagonal contribution in the

semiclassical approach, and we spend some time explaining how in the limit of clean systems the Nonlinear Sigma Model loses some non-perturbative information, correctly captured in the semiclassical calculations. Experimentally relevant results will be presented in chapter VII where we will show applications of our ideas in the realm of mesoscopic physics (distribution of decay widths in almost closed quantum dots and distribution of conductances in the Coulomb-Blockade regime).

In chapter VIII we summarize our results and offer a brief discussion of the fundamental open question concerning the statistical description of eigenfunctions in the semiclassical limit: the construction of the eigenfunction's probability distribution and the justification of the Gaussian conjecture.

## Chapter 2

# The statistical description of chaotic eigenfunctions

In this chapter we will introduce the basic concepts and available methods to describe statistically eigenfunctions in classically chaotic systems. Both averages and fluctuations can be calculated using different techniques depending on the problem at hand.

As expected, the possibility of using statistical techniques leads to a drastic simplification of the theory and to a substantial decrease of the classical information required. More importantly, it is almost invariably the case that the physics of the quantity under study already involve some kind of average.

## 2.1 An example: The effect of interactions in irregular quantum dots

It would take long to quote the applications and advantages of the use of statistical techniques when dealing with irregular eigenfunctions (see, for example, [28] and references therein) so we will present a recent and very relevant application of this idea in the context of electronic interactions in mesoscopic systems [29]: the construction of the “Universal Hamiltonian”.

Consider a number of electrons in a clean quantum dot, usually modeled as a quantum billiard (a particle inside a bounded domain undergoing specular reflections at the boundaries). In second quantized form, the Hamiltonian

is given by

$$\hat{H} = \sum_i \epsilon_i \hat{c}_i^\dagger \hat{c}_i + \frac{1}{2} \sum_{i,j,k,l} V_{i,j,k,l} \hat{c}_i^\dagger \hat{c}_j \hat{c}_k^\dagger \hat{c}_l, \quad (2.1)$$

where  $\hat{c}_i^\dagger, \hat{c}_i$  create and annihilate a particle in the single-particle state  $\psi_i$  with energy  $\epsilon_i$  which we take as the states and energies of the non-interacting system. The interaction matrix elements are then given by

$$V_{i,j,k,l} = \int \int \psi_i(\vec{r}_1) \psi_j(\vec{r}_2) V(\vec{r}_1 - \vec{r}_2) \psi_k(\vec{r}_1) \psi_l(\vec{r}_2) d\vec{r}_1 d\vec{r}_2, \quad (2.2)$$

where  $V(\vec{r}_1 - \vec{r}_2)$  is the inter-particle interaction potential.

In an exact quantum calculation one then proceeds to represent this Hamiltonian in a complete basis in Fock space and diagonalizes the corresponding matrix. To see the ideas about statistics of eigenfunctions at work, we assume that the classical single-particle dynamics is chaotic. If this is the case, the single-particle eigenfunctions  $\psi_i$  do not have any characteristic spatial structure, since there are not tori to support them. Then we expect that in average (indicated by  $\langle \dots \rangle$  and to be fully specified in a moment) it is equally likely that they are positive or negative at given point,

$$\langle \psi_i(\vec{r}) \rangle = 0. \quad (2.3)$$

In this case, we expect that the only interaction matrix elements that significantly contribute to the Hamiltonian are those that are positive definite, namely those with two indices equal pairwise. Neglecting all other possible terms this “diagonal Hamiltonian” is given by

$$\hat{H}^d = \sum_i \epsilon_i \hat{c}_i^\dagger \hat{c}_i + \frac{1}{2} \sum_{i,j} V_{i,i,j,j} \hat{c}_i^\dagger \hat{c}_i \hat{c}_j^\dagger \hat{c}_j + \frac{1}{2} \sum_{i,j} V_{i,j,i,j} \hat{c}_i^\dagger \hat{c}_j \hat{c}_i^\dagger \hat{c}_j. \quad (2.4)$$

As it will be carefully explained in the next chapters, all theoretical approaches together with experimental results and numerical calculations show that there is a regime where any average that is bilinear in the eigenfunctions is given by Berry’s universal result,

$$\langle \psi_i(\vec{r}_1) \psi_i(\vec{r}_2) \rangle = \frac{1}{A} F(|\vec{r}_1 - \vec{r}_2|), \quad (2.5)$$

with an universal function  $F(x)$  and the system’s area  $A$ . In this regime we finally get an expression for the Hamiltonian which is universal (i.e. it does

not depend on the particular system), the so-called universal Hamiltonian:

$$\hat{H}^u = \sum_i \epsilon_i \hat{c}_i^\dagger \hat{c}_i + \frac{V_1}{2} \sum_{i,j} \hat{c}_i^\dagger \hat{c}_i \hat{c}_j^\dagger \hat{c}_j + \frac{V_2}{2} \sum_{i,j} \hat{c}_i^\dagger \hat{c}_j \hat{c}_i^\dagger \hat{c}_j, \quad (2.6)$$

where

$$V_1 = \frac{1}{A^2} \int \int V(\vec{r}_1 - \vec{r}_2) d\vec{r}_1 d\vec{r}_2, \quad (2.7)$$

$$V_2 = \frac{1}{A^2} \int \int V(\vec{r}_1 - \vec{r}_2) d\vec{r}_1 F^2(\vec{r}_1 - \vec{r}_2) d\vec{r}_2. \quad (2.8)$$

Despite its apparent simplicity, this Hamiltonian has been extremely successful to describe a variety of mesoscopic effects, like magnetization of small metallic particles [30] and average Coulomb-Blockade spacings [31]. This success is a confirmation of the basic assumptions about the statistical behavior of irregular wavefunctions. On the other hand, its failures, like the wrong results concerning the distribution of peak spacings in the Coulomb-Blockade regime [28] can be traced back to the strong approximations we have done.

We also mention that although the non-diagonal interaction matrix elements have no direct influence on the structure of the universal Hamiltonian, their fluctuations can drive a phase transition from the insulating to the metallic regime at zero temperature, as it was shown using Renormalization Group techniques in [32]. This highly non-trivial result is also based on statistical assumptions about the eigenfunctions, and clearly indicates the need for a better understanding of the kind of averages involved, the size of the fluctuations and the influence of finite size and non-universal effects, all of them motivations for our present work.

To start building a statistical theory of eigenfunctions we need to specify the statistical ensemble and the kind of statistical measures we are interested to calculate, depending on the problem at hand.

## 2.2 The different types of average

When we want to describe an eigenfunction statistically, we can distinguish three kinds of averages: spatial, spectral and over disorder. When and how to apply each of them is the subject of this chapter, but we recall that they are not exclusive and sometimes a suitable combination of different types of average will be justified and/or necessary.

### 2.2.1 Spatial average

Consider an eigenfunction  $\psi_l(\vec{r})$  corresponding to the  $l$ -th energy level of a single-particle system. Consider now a functional of the eigenfunction, for example its powers at given point  $\psi_l(\vec{r})^n$  (its average  $R_n^l(\vec{r}) = \langle \psi_l(\vec{r})^n \rangle$  is known as the  $n$ -th moment). The spatial average takes as ensemble the values of the quantity under study over a given region  $S$  of volume  $\Omega(S)$  around the observation point  $\vec{r}$ , so in this case the moments are defined as

$$R_n^{l,spa}(\vec{r}) = \frac{1}{\Omega(S)} \int_{S(\vec{r})} \psi_l(\vec{q})^n d\vec{q}. \quad (2.9)$$

A typical choice for the region  $S$  is a circle centered at  $\vec{r}$ . The definition is readily generalized to the case where the observable depends on the values of the wavefunction at different points.

Formally, the use of such an average is strongly limited by the following facts:

- the choice of the region  $S$  must respect the natural boundaries of the system, namely, the average procedure itself depends on the geometry of the confinement,
- by construction, spatially integrated quantities, like the inverse participation ratios, are automatically self-averaging and then non-fluctuating, and
- the corresponding probability distribution is defined as the probability to find a particular numerical value among the numbers  $\psi_l(\vec{r}_1), \dots, \psi_l(\vec{r}_m)$  for a given eigenfunction, not the probability to find a particular  $\psi(\vec{r})$  among certain subset of eigenfunctions.

### 2.2.2 The average over disorder

There are both theoretical and experimental situations where it is necessary and/or convenient to explicitly perform an average over realizations of some fictitious potential, usually called “disorder”. If the statistical properties of the ensemble of disorder potentials allow it, eventually such average can be exactly performed. The best (in the sense of tractable) statistical properties correspond as expected to an ensemble of scatters with Gaussian-like correlation (although other choices are possible).

The theory of disordered systems provides tools to calculate such averages. An elegant technique based on the use of supersymmetry methods leads to what is known as the Nonlinear Sigma Model, about which more will be said in next chapters.

We consider again as example the moments  $R_n^l(\vec{r})$ . Let us denote with  $\psi_l(\vec{r}; V_i)$  the  $l$ -th eigenfunction corresponding to the  $i$ -th realization of the disorder potential  $V_i$ , defined for example by the spatial location of the scatterers. In the case of average over disorder the moments are defined as

$$R_n^{l,dis}(\vec{r}) = \frac{1}{N} \sum_{i=1}^N \psi_l(\vec{r}; V_i)^n, \quad (2.10)$$

and the Nonlinear Sigma Model provides an exact expression to calculate them, at least in the semiclassical limit and when the number  $N$  of systems in the ensemble goes to infinity.

Despite the enormous success of the Nonlinear Sigma Model when dealing with disordered systems, it faces some problems:

- its applicability in the realm of clean (ballistic) systems, where we are interested in a single quantum system and the classical dynamics is not diffusive but Hamiltonian, still lacks formal support,
- the conjectured ballistic version of the theory, the Ballistic Sigma Model, has been used to (formally) calculate system-specific properties, but the results are expressed in terms of a classical object (the classical propagator) which turns out to be as difficult to study, or more, as the original quantum problem, and
- it fails to predict some contributions to the averages which have been found both numerically and experimentally (such contributions will be discussed in chapters VI and VII).

We will discuss these points in great detail in the next chapters.

### 2.2.3 Spectral average

In the case of clean systems, i.e. when we are dealing with single systems and not with a family of them, the only sensible choices for an average are the spatial one, discussed before, and the spectral one.



For the spectral average we introduce an energy window  $W = [e - \frac{\delta e}{2}, e + \frac{\delta e}{2}]$  containing  $N_W$  energy levels and satisfying  $\frac{\delta e}{e} \ll 1$ , a situation we can always achieve in the semiclassical limit. The spectrally averaged moments are then defined as

$$R_n^{W, spe}(\vec{r}) = \frac{1}{N_W} \sum_{E_l \in W} \psi_l(\vec{r})^n, \quad (2.11)$$

and, being careful about its compatibility with the condition  $\frac{\delta e}{e} \ll 1$ , the limit  $N_W \rightarrow \infty$  can be also considered.

The spectral average provides the most natural averaging in the case of single systems, and when it is allowed to be used, it has the following advantages:

- its definition is fully system-independent,
- it automatically respects the boundary conditions imposed to the eigenfunctions, and
- it can be easily supplemented with an extra spatial or disorder average when required.

From now on we will refer only to energy averages and the superscripts “*spe*” and “*W*” will be dropped, but note that by construction the spectral average depends on both the size of the energy window  $\delta e$  and the energy at its center  $e$ .

## 2.3 Some important statistical measures

There are some particular functionals of the wavefunction which, after averaging, provide statistical information that is easy to interpret and useful for practical calculations (we have already found one,  $R_n(\vec{r})$ ). Since we will refer to them very often, we present here the corresponding definitions.

The  $n$ -point spatial self-correlation function (or simply  $n$ -point correlation function) is defined as

$$\begin{aligned} R_n(\vec{r}_1, \dots, \vec{r}_n) &= \langle \psi(\vec{r}_1) \dots \psi(\vec{r}_n) \rangle \\ &= \frac{1}{N_W} \sum_{E_l \in W} \psi_l(\vec{r}_1) \dots \psi_l(\vec{r}_n). \end{aligned} \quad (2.12)$$

Of course all moments and cumulants are particular cases or combinations of such correlations. As we will see, the two-point case ( $n = 2$ ), denoted simply by  $R(\vec{r}_1, \vec{r}_2)$  and given by

$$\begin{aligned} R(\vec{r}_1, \vec{r}_2) &= \langle \psi(\vec{r}_1) \psi(\vec{r}_2) \rangle \\ &= \frac{1}{N_W} \sum_{E_l \in W} \psi_l(\vec{r}_1) \psi_l(\vec{r}_2), \end{aligned} \quad (2.13)$$

will play an important role.

Other measures are related to the full distribution of the intensities  $(\psi(\vec{r})^2)$  and its spatial correlations. We define then

$$\begin{aligned} I_n(w_1, \dots, w_n, \vec{r}_1, \dots, \vec{r}_n) &= \langle \delta(w_1 - \psi(\vec{r}_1)^2) \dots \delta(w_n - \psi(\vec{r}_n)^2) \rangle \\ &= \frac{1}{N_W} \sum_{E_l \in W} \delta(w_1 - \psi_l(\vec{r}_1)^2) \dots \delta(w_n - \psi_l(\vec{r}_n)^2). \end{aligned} \quad (2.14)$$

Note that they all depend on the particular set of points where the spectral average is taken and on the size and location of the energy window  $W$ .

## 2.4 Theoretical approaches

In this section we will present the available techniques to describe the statistical properties of irregular eigenfunctions in the semiclassical regime.

Once the kind of average is defined, the final goal of any statistical approach is to construct the corresponding functional probability distribution  $P[\psi(\vec{r})]$ , defined as

$$\begin{aligned} P[\psi(\vec{r})] \mathcal{D}[\psi] \\ = \\ \text{probability to find an eigenfunction between} \\ \psi(\vec{r}) \text{ and } \psi(\vec{r}) + d\psi(\vec{r}). \end{aligned} \quad (2.15)$$

As expected, however, the full determination of this object from basic principles is in general an impossible task. There is not a single quantum system where the probability distributions can be derived in terms of a closed expression (unless, of course, the whole set of eigenfunctions is known).

As was mentioned in the introduction, having highly sophisticated methods to deal with the precise and particular structure of individual eigenfunctions (like the Fredholm method or the explicit numerical calculation) is not very helpful, since the jump to the desired averages then involves an extra complication instead of reducing the amount of work and information. This is particularly obvious when dealing with universal properties; the statistical theory must provide a scheme where universal properties appear naturally (instead of being an obscure result coming from magic cancellations of the particular features among the different members of the ensemble). So, while giving microscopic support to the statistical theory by means of ergodic theorems is in general a formidable task, a suitable, physically motivated choice of the distribution probability must be considered as an option.

A usual procedure is to replace the ensemble under study by another ensemble which is constructed under physically motivated assumptions and respects the possible constraints we can incorporate without rendering the model intractable. This is the basic idea behind the so-called Random Wave Models, which have constituted the method par excellence for the statistical description of chaotic wavefunctions since Berry's pioneering work in 1977 [20].

Because of their importance, we start our description of the available methods with an historical and conceptual review of the Random Wave Models. The story begins with the discovery of the universal two-point correlation function.

### **2.4.1 The Voros-Wigner function and the universal two-point correlation function**

The extremely rich spatial pattern of wavefunctions in classically chaotic systems was discovered for the first time by McDonald and Kaufmann in 1979 in their numerical exploration of high lying states in the Bunimovich billiard, a known example of a classically chaotic system [33]. However, the first theoretical techniques were developed some years earlier by Berry in 1977 [20], following a suggestion made in 1967 by Voros [34].

The basic ingredient of the theory is the Wigner function associated with the eigenfunction  $\psi_l(\vec{r})$ , defined as (we restrict ourselves to the 2-D case,

there are no new conceptual ingredients in higher dimensions) [35]

$$\Psi_l(\vec{r}, \vec{p}) = \frac{1}{(2\pi\hbar)^2} \int_{\Omega} e^{-\frac{2i}{\hbar} \vec{p} \cdot \vec{R}} \psi_l(\vec{r} + \vec{R}) \psi_l(\vec{r} - \vec{R}) d\vec{R}, \quad (2.16)$$

where the integral runs over the whole configuration space of the system.

The Wigner function is the quantum mechanical version of the phase space density in classical statistical mechanics, and in fact this was the initial motivation of Wigner to introduce it. This analogy must be taken with care, however, since  $\Psi_l$  can become negative. For a comprehensive review of the phase space formalism in quantum mechanics and its applications, see [35].

The Wigner function can be used to obtain, via Fourier transform, the two-point correlation function as [20]

$$\langle \psi_l(\vec{r} + \vec{R}) \psi_l(\vec{r} - \vec{R}) \rangle = \frac{1}{(2\pi\hbar)^2} \int_{\Omega} e^{\frac{2i\vec{p} \cdot \vec{R}}{\hbar}} \langle \Psi_l(\vec{r}, \vec{p}) \rangle d\vec{p}. \quad (2.17)$$

The only strong mathematical result about the averaged Wigner function  $\langle \Psi_l(\vec{r}, \vec{p}) \rangle$  was put forward by Shnirelman in a celebrated result referred to as the quantum ergodicity theorem [36]: For systems with ergodic classical dynamics (which is a necessary condition for chaos), the sequence  $\langle \psi_l | \hat{A} | \psi_l \rangle$  for any quantum observable  $\hat{A} = A(\hat{r}, \hat{p})$  converges to the classical micro-canonical average in the  $E_l \rightarrow \infty$  limit,

$$\langle \psi_l | \hat{A} | \psi_l \rangle \rightarrow \frac{1}{\Sigma^*(E_l)} \int_{\Omega^*} \delta(H(\vec{r}, \vec{p}) - E_l) A(\vec{r}, \vec{p}) d\vec{r} d\vec{p}. \quad (2.18)$$

where  $\Omega^*$  is the classical phase space and  $\Sigma^*(E_l) = \int_{\Omega^*} \delta(H(\vec{r}, \vec{p}) - E_l) d\vec{r} d\vec{p}$  is the volume of the classical energy shell.

It can be formally proven that in the phase-space formalism of quantum mechanics, the expected values can be written in terms of the Wigner function as

$$\langle \psi_l | \hat{A} | \psi_l \rangle = \int_{\Omega^*} \Psi_l(\vec{r}, \vec{p}) A_W(\vec{r}, \vec{p}) d\vec{r} d\vec{p} \quad (2.19)$$

with a well defined mapping  $A(\hat{r}, \hat{p}) \rightarrow A_{\text{Weyl}}(\vec{r}, \vec{p}) = A(\vec{r}, \vec{p}) + O(\hbar)$  [35] ( $A_{\text{Weyl}}(\vec{r}, \vec{p})$  is called “Weyl symbol” of the operator  $\hat{A}$ ). This result suggests that in the semiclassical limit, when  $E_l$  is finite, the average Wigner function can be approximated as

$$\langle \Psi_l(\vec{r}, \vec{p}) \rangle \rightarrow \frac{1}{\Sigma^*(E_l)} \delta(H(\vec{r}, \vec{p}) - E_l), \quad (2.20)$$

with the limit understood in the weak sense. We remark that this last expression has not been rigorously derived, and in particular it is not known which kind of average it implies, but it is very well sustained by both theoretical and numerical calculations at least in the spectral average case.

For a system with two degrees of freedom that is governed by the Hamiltonian  $H(\hat{r}, \hat{p}) = \hat{p}^2/2m + V(\hat{r})$ , we obtain from Eq. (2.17)

$$\langle \psi_l(\vec{r} + \vec{R}) \psi_l(\vec{r} - \vec{R}) \rangle = \frac{1}{A(e)} J_0 \left( |\vec{R}| \sqrt{\frac{2m(e - V(\vec{r}))}{\hbar}} \right), \quad (2.21)$$

with  $A(e) = \int_{V(\vec{r}) < e} d\vec{r}$  the accessible area in configuration space,  $e \sim E_l$ , and  $J_0(x)$  is the Bessel function.

This fundamental result, put forward for the first time by Berry [20] is the cornerstone of the theory of eigenfunctions in chaotic systems, and has been successfully applied to a large variety of systems and situations [37]. It expresses the universality of the two-point correlation function since it is independent of the particular system under study and gives the promised support to the universal Hamiltonian (see section 2.1).

On the other hand, the two-point spatial correlation function (universal or not) is not enough to fully characterize the statistical properties of the wavefunction, as it is clear by considering any measure involving higher order products, like any higher-order correlation function. At this point we must forget about formal results and consider some kind of statistical model.

### 2.4.2 The isotropic Random Wave Model

In his 1977 paper, Berry went a step further by realizing that the universal two-point correlation function, *is exactly the same as the one of a random superposition of plane waves* with local wavenumber  $k = \sqrt{2m(e - V(\vec{r}))}/\hbar$ . To keep the presentation simple, we consider from now on billiard systems with area  $A$  (i.e.  $k$  is independent of the position). Consider now the random function

$$\psi^{RWM}(\vec{r}) = \frac{1}{\sqrt{AJ}} \sum_{j=1}^J \cos(k\vec{\theta}_j \cdot \vec{r} + \delta_j) \quad (2.22)$$

with  $\delta_1, \dots, \delta_J$  a set of  $J$  ( $\gg 1$ ) independent random variables uniformly distributed over  $(0, 2\pi]$ . If the directions of the waves are also taken as

uniformly distributed over the unit circle, i.e.

$$\vec{\theta}_j = \left( \cos \frac{2j\pi}{J}, \sin \frac{2j\pi}{J} \right), \quad (2.23)$$

the two-point correlation is, after average over  $\delta_1, \dots, \delta_J$ ,

$$R^{RWM}(\vec{r}_1, \vec{r}_2) = \frac{1}{AJ} \sum_{j=1}^J \cos(k\vec{\theta}_j \cdot (\vec{r}_1 - \vec{r}_2)) \quad (2.24)$$

which in the limit  $J \rightarrow \infty$  gives exactly Eq. (2.21),

$$R^{RWM}(\vec{r}_1, \vec{r}_2) = \frac{1}{A} J_0(k|\vec{r}_1 - \vec{r}_2|) \quad (2.25)$$

Simple arguments based on the central limit theorem were put forward in order to consider the different values of a given eigenfunction as independent Gaussian variables, while an exact mathematical result states that the random superposition Eq. (2.22) above is also a Gaussian field.

In this way, an interesting connection between the statistical properties of irregular eigenfunctions and a random superposition of plane waves has been established: they have roughly the same global statistical distribution (Gaussian) and exactly the same two-point correlation function under suitable averaging (Bessel). *Statistically speaking they are the same theory.*

Although it is extremely difficult to relax the Gaussian structure of the theory in order to include system dependent effects (which are completely neglected in the isotropic Random Wave Model), much more can be done at the level of the two-point correlation function, as we explain in the following. The theories defined as Gaussian fields but using a different basis for the random superposition (instead of the plane waves), are the non-isotropic Random Wave Models.

### 2.4.3 The non isotropic Random Wave Models

It is clear that the ergodic result for the correlation function can only reproduce the gross spatial features of the wavefunction. In fact, it predicts a constant value for the average intensity,

$$R^{RWM}(\vec{r}, \vec{r}) = \frac{1}{A} \quad (2.26)$$

in contrast to the actual behavior shown in Fig. (3.2). Generally speaking, all possible effects related to the existence of boundaries in the classical motion are not properly taken into account in the ergodic approximation. This happens already at the level of the simplest statistical measure, the two-point correlation. Of course this is not a surprise since Berry's expression is universal and fully independent of the particular structure of the confinement.

It took almost 30 years before Berry [38, 39], Heller and Lepore [40], and Heller and Biess [41] developed suitable modifications to the Random Wave Model which adequately incorporate some kind of highly idealized boundaries. The first Berry's non-isotropic Random Wave Models [38] assumes an infinite linear boundary along which Dirichlet or Neumann boundary conditions are demanded, and builds random superpositions of plane waves that are adapted to this new constraint.

Consider a boundary that is locally approximated as the straight infinite line

$$y = y_0 \quad (2.27)$$

with  $y_0 > 0$ . Let  $y < y_0$  be the "interior" of the system. An ensemble of random superpositions of plane waves satisfying Dirichlet (D) boundary conditions along the line

$$\psi_D^{RWM}(\vec{r})|_{y=y_0} = 0 \quad (2.28)$$

is easily constructed using the method of images. Taking  $\vec{r} = (x, y)$ , it is given by

$$\psi_D^{RWM}(x, y) = \frac{1}{2}(\psi^{RWM}(x, y) - \psi^{RWM}(x, 2y_0 - y)), \quad (2.29)$$

while the ensemble for Neumann (N) boundary conditions

$$\frac{\partial \psi_N^r(\vec{r})}{\partial y}|_{y=y_0} = 0 \quad (2.30)$$

is given in analogy by

$$\psi_N^{RWM}(x, y) = \frac{1}{2}(\psi^{RWM}(x, y) + \psi^{RWM}(x, 2y_0 - y)), \quad (2.31)$$

We note that what we are doing is merely projecting the isotropic random wave function  $\psi^{RWM}(\vec{r})$  over the two invariant subspaces of the symmetry group (describing the reflection symmetry of the system with respect

to  $y = y_0$ ) by means of the corresponding projectors. This immediately suggests a generalization to the symmetry group associated with the rotations with angle  $\pi/n$  with  $n = 1, 2, \dots$  in order to construct a non-isotropic Random Wave Model for a “wedge” boundary [40]. The physics of this general ensemble does not introduce any new feature, so we keep the presentation simple by considering now the  $n = 1$  case originally studied by Berry.

Explicit substitution of the random superposition Eq. (2.22), and averaging over the same set of random coefficients and phases gives for the two point correlation function,

$$\begin{aligned} R_{D,N}^{RWM}(\vec{r}_1, \vec{r}_2) &= \frac{1}{A} J_0 \left( k \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2} \right) \\ &\mp \frac{1}{A} J_0 \left( k \sqrt{(x_1 - x_2)^2 + (y_1 + y_2 - 2y_0)^2} \right). \end{aligned} \quad (2.32)$$

The generalization for the wedge case is then straightforward. With this expression for the two-point correlation and assuming the statistics to be Gaussian, one has a full statistical theory.

In particular, we note that the average intensity is no longer constant and exhibits oscillations reflecting quantum interference effects produced by the boundary:

$$R_{D,N}^{RWM}(\vec{r}, \vec{r}) = \frac{1}{A} (1 \pm J_0(2k|y - y_0|)), \quad (2.33)$$

The basic ideas presented before were further generalized to incorporate more general boundary conditions as well as the case where the potential barrier is smooth instead of hard. For completeness and to fix notation we present also these developments.

#### 2.4.4 Further extensions of the Random Wave Model

A highly non-trivial generalization of the non-isotropic Random Wave Model in the presence of an infinite straight barrier is achieved by imposing the more general (hermitian) mixed (M) boundary conditions along  $y = y_0 = 0$  [39],

$$\left( k\psi_M^{RWM}(\vec{r}) \cos \alpha + \frac{\partial \psi_M^{RWM}(\vec{r})}{\partial y} \sin \alpha \right) |_{y=y_0=0} = 0, \quad (2.34)$$

where  $\alpha$  is a parameter interpolating between the Dirichlet ( $\alpha = 0$ ) and Neumann ( $\alpha = \pi/2$ ) cases. Introducing

$$f_\alpha(y, \theta) = \frac{\cos \alpha \sin(ky \sin \theta) - \sin \alpha \sin \theta \cos(ky \sin \theta)}{\sqrt{\cos^2 \alpha + \sin^2 \alpha \sin^2 \theta}}, \quad (2.35)$$



the corresponding ensemble is easily verified to be

$$\psi_M^{RWM}(\vec{r}) = \frac{2}{\sqrt{AJ}} \sum_{j=1}^J f_\alpha(y, \theta_j) \cos(kx \cos \theta_j + \delta_j). \quad (2.36)$$

The usual average over the phases and the limit  $J \rightarrow \infty$  gives the correlation function:

$$R_M^{RWM}(\vec{r}_1, \vec{r}_2) = \frac{1}{2\pi A} \int_0^{2\pi} f_\alpha(y_1, \theta) f_\alpha(y_2, \theta) \cos(k(x_1 - x_2) \cos \theta) d\theta, \quad (2.37)$$

and the corresponding average intensity

$$R_M^{RWM}(\vec{r}, \vec{r}) = \frac{1}{2\pi A} \int_0^{2\pi} f_\alpha^2(y, \theta) d\theta. \quad (2.38)$$

For more general situations where the confining potential is smooth (S), Bies and Heller [41] idealized the boundary as a linear ramp potential  $V(x, y) = V_0 y$ . The following random superposition is easily shown to satisfy locally the Schrödinger equation for the linear ramp:

$$\psi_S^{RWM}(\vec{r}) = \frac{1}{\sqrt{AJ}} \sum_{j=1}^J \text{Ai}[\Psi(y, Q_j)] \exp[i(Q_j x + \delta_j)], \quad (2.39)$$

where

$$\Psi(y, Q) = \left(\frac{V_0}{\hbar^2}\right)^{\frac{1}{3}} (y - y_0) + \left(\frac{\hbar^2}{V_0}\right)^{\frac{2}{3}} Q^2, \quad (2.40)$$

$y_0 = e/V_0$  is the turning point fixed by the mean energy  $e$  of the eigenstates under study, and  $\text{Ai}(x)$  is the Airy function.

The phases  $\delta_j$  provide the averaging, while  $Q_j \in [-\infty, \infty]$ . Explicit calculation then gives for the two point correlation function:

$$R_S^{RWM}(\vec{r}_1, \vec{r}_2) = \left(\frac{2\pi^3}{\hbar^4 V}\right)^{\frac{1}{3}} \int_0^\infty \cos(Q(x_1 - x_2)) \times \text{Ai}\left[\left(\frac{V}{\hbar^2}\right)^{\frac{1}{3}} \left(y_1 - \frac{E - \hbar^2 Q^2}{V}\right)\right] \text{Ai}\left[\left(\frac{V}{\hbar^2}\right)^{\frac{1}{3}} \left(y_2 - \frac{E - \hbar^2 Q^2}{V}\right)\right] dQ, \quad (2.41)$$

and for the average intensity,

$$R_S^{RWM}(\vec{r}, \vec{r}) = \int_0^\infty \text{Ai}^2[\Psi(y, Q)] dQ. \quad (2.42)$$

With this ensemble we finish the presentation of all known Random Wave Models. The Gaussian structure of the theories together with the two-point correlation functions provide a full statistical description of the corresponding ensemble.

### 2.4.5 Final remarks about the Random Wave Models

As we carefully stressed in the last sections, the conceptual foundations of the Random Wave Models can be directly traced back to the initial semiclassical evaluation of the universal two-point correlation function by Berry.

This point of view, however, was soon left aside by the most practical implementation which is based on the random superposition of some particular class of basis functions. This change of perspective had an immediate consequence; it moved the focus into the construction of models, instead of the derivation from first principles of the Gaussian distribution and the correlation function.

We believe that the basic motivations behind the introduction of the Random Wave Model must be recovered and efforts should be focused on two basic aims:

- A full microscopic theory of the two-point correlation function independent of any statistical assumption or ensemble would be desirable. Such theory must explain the success of both the isotropic and non-isotropic Random Wave Model at the level of the two-point case.
- A full microscopic derivation of the wavefunction probability distribution in order to keep the Gaussian approximation under control.

Presently we know how to carry on the first part of this program, and a huge amount of evidence (experimental, numerical and theoretical) supports the Gaussian approximation for the wavefunction distribution. The microscopic justification of the Random Wave Models and its success is still an object of research.

Now we turn our attention to another, completely different approach to the problem, a heritage coming from the success of supersymmetry methods in the statistical description of eigenfunctions in disordered systems.

### 2.4.6 The Nonlinear Sigma Model

The purpose of the Random Wave Model is the statistical description of eigenfunctions in *clean and classically chaotic systems*, which is the main interest of the present work. There is, however, an extremely powerful technique developed for the statistical description of eigenfunctions in *classically diffusive systems*, which has been extended to describe also the clean (ballistic) case. The name of this approach, Nonlinear Sigma Model, is taken from the effective field theory it produces as a mapping of the original problem.

In this section we very briefly present the physical motivations (averaging over disorder), the mathematical methods (supersymmetry techniques), and the general structure of the results of this approach (in terms of the classical diffusive propagator). The presentation will be kept at a minimum of complexity. The reader is referred to the many excellent introductions to the subject [42, 43].

Consider a disordered system described by the Hamiltonian  $\hat{H}_\alpha = H(\hat{p}, \hat{r}) + V_\alpha(\hat{r})$ . For a given realization  $V_\alpha(\vec{r})$  of the disorder potential, any combination of eigenfunctions can be expressed in terms of the system's Green function

$$G_{V_\alpha}(\vec{r}_1, \vec{r}_2, z) = \langle \vec{r}_1 | (H(\hat{p}, \hat{r}) + V_\alpha(\hat{r}) - z)^{-1} | \vec{r}_2 \rangle. \quad (2.43)$$

Typically, statistical measures, when averaged over disorder, depend on the evaluation of expressions like

$$\int \left[ \prod_{i,j} G_V(\vec{r}_i, \vec{r}_j, z) \right] P(V) dV, \quad (2.44)$$

where  $P(V)$  is the probability distribution of the disordered potential. Looking for an efficient and well controlled way to calculate such integrals is the ultimate motivation of the supersymmetry techniques in the theory of disordered systems.

Contrary to some previous efforts (the so-called replica trick and perturbation theory), the introduction of Grassmann (anticommuting) variables by Efetov [42] permits an *exact* calculation of the average over the disorder potential. This is achieved by a nice mathematical property of the Grassmann integrals that lifts the complicated denominators appearing in the Green function. The disorder potential is placed in the exponent, which permits an explicit integration, at least in the very common case of white-noise correlated and Gaussian distributed disorder. After performing the average over

disorder (which can be done analytically), one is left with a field theory (the Nonlinear Sigma Model) which can be treated with all the available techniques (perturbation theory, renormalization group, saddle-point and instanton approximations, etc).

The amazing success of the Nonlinear Sigma Model is based on the fact that both the mapping of the original problem and the calculation of the average over disorder are done exactly. In this way, a very deep understanding of the physics of disordered media has been achieved, even in regimes where standard techniques were difficult (or even not allowed) to be used, like the limit of strong disorder where Anderson localization takes place, and the metal-insulator transition where the eigenfunctions display fractal features. Even more, the universal contributions to the statistical measures given by the Nonlinear Sigma Model have been formally proven to be the predictions of the Random Matrix Theory, giving formal support to the application of RMT to derive universal results in disordered systems.

Being a semiclassical theory, the deviations from universality obtained by the use of the Nonlinear Sigma Model are typically expressed in terms of classical objects. Since the classical limit of a disordered system is Brownian motion, the results are then expressed in terms of (maybe very complicated) functions of the *classical diffusive propagator*, a pure classical object calculated by solving the diffusive equation with suitable boundary conditions (see the appendix). From the well-known properties of this propagator, the theory can make precise predictions about system-specific properties.

With such a successful theory at hand, the obvious question arose about its possible generalization to describe clean systems, where in principle no average over disorder is justified. However, we have seen that the average over disorder is an essential ingredient of the theory and the transition to a theory describing clean systems is far from obvious. Presently there is no agreement among experts in the field about how to correctly take this “zero disorder” limit, but a number of increasingly more complicated steps have been taken in order to provide a ballistic version of the Nonlinear Sigma Model [45, 66].

In practice, all different proposals coming from the theory of disordered systems end with a simple and direct recipe to calculate statistics of eigenfunctions in the clean chaotic case: take the results of the usual Nonlinear Sigma Model *in the metallic regime* (there is no Anderson-type localization in clean systems) and substitute the classical diffusive propagator by its Hamiltonian counterpart, called Liouville propagator. However, as shown in the

appendix, the diffusive propagator is defined only in configuration space, while the Hamiltonian propagator is defined in phase space. Hence, *the Ballistic Sigma Model predicts the results of the Nonlinear Sigma Model for the metallic regime, where the diffusive propagator is substituted by the projection on configuration space of the classical Liouville propagator.*

We will provide specific results of the Ballistic Sigma Model when we discuss its relation with the semiclassical approach in chapter VI, but by now we can be more explicit about first the criticism presented in section 2.2.2 concerning the use of the Sigma Model techniques in clean systems: in contrast to the diffusive case, almost nothing is known about the Liouville propagator and the methods to construct its (highly singular) spatial properties. In general, the (numerical) construction of the Liouville propagator in chaotic systems is even more difficult than the explicit numerical solution of the Schrödinger equation.

The two-point correlation function obtained from the Sigma Model does not differ from the one resulting from the Random Wave Model. The corresponding results read [28]

$$R^\sigma(\vec{r}_1, \vec{r}_2) = \frac{1}{A} J_0(k|\vec{r}_1 - \vec{r}_2|), \quad (2.45)$$

and for the average intensity [31]

$$R^\sigma(\vec{r}, \vec{r}) = \frac{1}{A}. \quad (2.46)$$

This results then explain our second criticism of section 2.2.2. In the same way as the isotropic Random Wave Model, the Sigma Model results do not reproduce the oscillatory contributions coming from quantum interference due to the boundary, which are displayed e.g. in Figure (3.1).

Since the two-point correlation function completely determines a Gaussian theory, and since the Sigma Model results for such function are just the universal results from the Random Wave Model, the Nonlinear Sigma Model includes non-universal effects by modifying the Gaussian distribution (which is a highly non-trivial task [66]).

Now we turn to the construction of the advertised semiclassical theory and discuss its two basic ingredients: the semiclassical two-point correlation function and the Gaussian conjecture.

## Chapter 3

# The semiclassical two-point correlation function

In this chapter we present a microscopic derivation of the semiclassical expression for the (energy averaged) two-point spatial correlation function. The result is valid for arbitrary potentials and boundary conditions, but for simplicity we will focus, as usual, on two-dimensional (2-D) systems with real eigenfunctions. Although many results will appear familiar, contrary to the basic assumptions of the Random Wave Models *no statistical assumption about the wavefunction will be made*.

### 3.1 Connecting the two-point correlation and the Green function

To remember, we define the (energy averaged) two-point correlation function as

$$R(\vec{r}_1, \vec{r}_2) = \frac{1}{N_W} \sum_{E_l \in W} \psi_l(\vec{r}_1) \psi_l(\vec{r}_2) \quad (3.1)$$

where  $W$  is an energy interval  $[e - \delta e/2, e + \delta e/2]$  containing  $N_W$  non-degenerate energy levels. Our starting point is the exact quantum mechanical representation of the Green function in terms of the eigenfunctions and eigenvalues:

$$G(\vec{r}_1, \vec{r}_2, z) = \sum_l \frac{\psi_l(\vec{r}_1) \psi_l(\vec{r}_2)}{z - e_l} \quad (3.2)$$

from which, by using the identity

$$\frac{1}{x + i0^+} - \frac{1}{x - i0^+} = -2i\pi\delta(x), \quad (3.3)$$

one gets a relation between the correlation and Green functions

$$R(\vec{r}_1, \vec{r}_2) = \frac{1}{\pi N_W} \int_{e-\delta e/2}^{e+\delta e/2} \text{Im} [G(\vec{r}_1, \vec{r}_2, E + i0^+)] dE. \quad (3.4)$$

This is the fundamental equation of this chapter. Being an exact result, it is clearly valid in any closed system with any kind of boundary conditions.

As expected, Eq. (3.4) above is of limited practical use as it stands, since it assumes the prior knowledge of the exact Green function of the system. It is, however an excellent starting point to introduce approximations, since we have a good variety of methods to approximate the Green function in different situations. The preferred method to be used in this work is the semiclassical approach based on the semiclassical Green function.

The semiclassical Green function is given in terms of the classical paths  $\gamma_{i,j}$  connecting the positions  $\vec{r}_i, \vec{r}_j$  with a given complex energy  $z = e + i0^+$  [7]

$$G^{sc}(\vec{r}_i, \vec{r}_j, z) = \frac{1}{i\hbar\sqrt{2\pi\hbar}} \sum_{\gamma_{i,j}} \sqrt{|D_{\gamma_{i,j}}(\vec{r}_i, \vec{r}_j, e)|} e^{\frac{i}{\hbar} S_{\gamma_{i,j}}(\vec{r}_i, \vec{r}_j, z) - i\mu_{\gamma_{i,j}} \frac{\pi}{2}}, \quad (3.5)$$

For each trajectory  $\gamma_{i,j}$  we must then compute

- its action  $S_{\gamma_{i,j}}(\vec{r}_i, \vec{r}_j; e) = \int_{\gamma_{i,j}} \vec{p} \cdot d\vec{q}$ ,
- its stability matrix  $M(\vec{r}_i, \vec{r}_j; e)$  (the linear mapping connecting small variations in phase space perpendicular to the trajectory at time 0 with those at time  $T_{\gamma_{i,j}}$ ) which gives the semiclassical amplitude  $D_{\gamma_{i,j}} = (|\dot{\vec{r}}_i| |\dot{\vec{r}}_j| |M_{1,2}|)^{-1}$ , and
- the number of conjugate points which gives an extra phase  $\mu_{\gamma_{i,j}}$ .

What is left is of course trivial: substitution of the semiclassical Green function into Eq. (3.4). The fact that the energy interval considered is by definition small in classical scales (more precisely we are assuming  $\frac{S_{\gamma_{i,j}}(E)}{T_{\gamma_{i,j}}(E)} \gg \delta e$  with  $T_{\gamma_{i,j}} = \frac{\partial S_{\gamma_{i,j}}(E)}{\partial E}$  the flight time of the trajectory) allows us to expand

the actions in the exponentials to first order and to take the amplitudes evaluated at the center of the window, since they are all smooth functions of the energy. The resulting two-point correlation function is then  $R^{sc}(\vec{r}_i, \vec{r}_j) = A(e)^{-1}(\delta_{i,j} + \tilde{R}(\vec{r}_i, \vec{r}_j))$  with the oscillatory contribution given by

$$\tilde{R}(\vec{r}_i, \vec{r}_j) = \sum_{\gamma_{i,j}} \Gamma\left(\frac{T_{\gamma_{i,j}}}{\tau_W}\right) \left| \frac{2\hbar}{\pi m^2} D_{\gamma_{i,j}} \right|^{1/2} \cos\left(\frac{S_{\gamma_{i,j}}}{\hbar}\right) \quad (3.6)$$

with a window function  $\Gamma(x) = \sin(x)/x$  that effectively cancels contributions from paths with traversal time  $T_{\gamma_{i,j}}$  larger than the characteristic time  $\tau_W = 2\hbar/\delta e$ .

The error we make by using the semiclassical approximation is bounded by the following formal result [7]:

$$R(\vec{r}_i, \vec{r}_j) = R^{sc}(\vec{r}_i, \vec{r}_j) + O(\hbar_{eff}^{3/2}), \quad (3.7)$$

which, together with the fact that the semiclassical correlation function scales as

$$\tilde{R}^{sc}(\vec{r}_i, \vec{r}_j) \sim O(\hbar_{eff}^{1/2}), \quad (3.8)$$

bounds the order of the expressions we can safely calculate using the semiclassical approach.

### 3.1.1 The universal contribution to the correlation function (again)

The semiclassical correlation function was constructed by means of the semiclassical Green function which in turn is based on a stationary phase approximation of the Feynmann propagator. As usual, the semiclassical approximation requires the actions of the classical paths involved to be much larger than  $\hbar$ , but this condition obviously fails when the two points in the argument of the propagator are too close to each other, since for short distances the action is simply proportional to the distance  $|\vec{r}_i - \vec{r}_j|$ . In order to solve this problem one can use the exact short-time quantum propagator, together with the formula connecting the Green function with the correlation to describe the short-path contribution  $R^{is}(|\vec{r}_i - \vec{r}_j|)$ , where “*is*” means that the result is isotropic, i.e., depending only on the distance between the points.



Since in 2D systems the short time Green function is given by  $i/4m$  times the Hankel function [7]  $H_0(k|\vec{r}_i - \vec{r}_j|) = J_0(k|\vec{r}_i - \vec{r}_j|) - iY_0(k|\vec{r}_i - \vec{r}_j|)$  with  $k = \sqrt{\frac{2m(e-V(\vec{r}_i))}{\hbar}}$ , a simple calculation then yields [46]:

$$R^{is}(|\vec{r}_i - \vec{r}_j|) = \frac{1}{A(e)} J_0(k|\vec{r}_i - \vec{r}_j|). \quad (3.9)$$

We remark that this result is quantum mechanically exact for constant potential or, thinking semiclassically, as long as one neglects the effect of classical paths with turning points. It is, again, the well known result predicted by Berry. Basically the same derivation has been presented in [47, 48]. A formula connecting smoothly the short (Bessel) and large (Eq. (3.6)) distance expressions for the correlation can be derived using uniform approximation techniques to the propagator [48], but in our experience such intermediate regime is hardly accessible.

The contribution from longer classical paths, in particular from paths with one or more turning points, depends on the particular structure of the confinement potential and then is neither isotropic nor universal. Although such contributions are known to exist and have been briefly studied before, their effect in the statistical measures beyond the two-point correlation has been never considered and is the main topic of this work.

How relevant are the non-universal contributions to the statistical description of irregular eigenfunctions?... it depends on the type of average performed. When the energy average is supplemented with an extra spatial average, the isotropic result turns out to be of leading semiclassical order compared with the non-universal contribution, as shown in [49]. This is one of the reasons why it was believed that the non-universal contribution could be neglected. Since in our theory we are not using so far any extra spatial average, both universal and non-universal contributions are of the same order in  $\hbar_{eff}$ .

Now we will provide numerical evidence of the existence of the non-universal effects at the level of the two-point correlation function.

### 3.1.2 Numerical and experimental tests of the semiclassical prediction for the correlation function

The universal part of the correlation function has been tested either directly or by means of its statistical implications in several works [37]. In the meso-

scopic realm, however, such experiments are very difficult to realize and the available results typically required an extra spatial average, washing away the non-universal contributions we want to study.

Another option is to use an exact mapping between the Schrödinger equation for billiard systems and the Helmholtz equation in the case of microwave cavities [50]. In the microwave case the measurement of high-lying eigenstates can be done with great accuracy and this sort of experiments have become very popular to check the predictions of theoretical models. The experimental results show an impressive agreement with the Bessel-like correlation function but, as mentioned before, this is to be expected when spatial averages are taken, as it is almost invariably the case.

Numerical tests of the theory at the universal level are also available, confirming the correctness of the Bessel result when both energy and spatial averages are used [51]. To our knowledge the only systematic study of the structure of the correlation function beyond the universal regime when only spectral averages are considered is presented here [49].

The specific system we study is the so called Africa billiard, obtained by a conformal deformation of the unit circle [52]. The reason to use such billiard is that it is easy to handle numerically and it can be modeled experimentally [50]. The exact correlation functions are obtained by explicit calculation of the eigenfunctions up to the 300-th energy level and use of the definition Eq. (3.1) with an energy window satisfying the semiclassical requirements and such that  $\tau_W$  is of the order of the traveling time through the system (so-called Thouless time). Due to the damping function  $\Gamma$ , this allows us to keep in the semiclassical two-point correlation function only classical paths with at most one bounce with the boundary.

The semiclassical calculations, when naively applied, gave very bad results except in a region very close to the boundary. After examination, it turned out that this system has a very problematic optical structure, namely, much of the billiard's domain is affected by effects beyond the ray-description which is the optical analogue of the semiclassical approximation. Such deviations from the ray-picture are called in general *diffraction effects* [53], and almost all of them are present in our system (penumbra effects, caustics, focal points, etc).

To overcome this problem, we include diffraction effects in the semiclassical expression for the two-point correlation function with paths up to one bounce to the boundary. This is achieved by calculating the full diffraction integral in the vicinity of each classical trajectory involved in Eq. (3.6). This

is done by means of the expression [54]

$$R^{sc+dif}(\vec{r}_i, \vec{r}_j) = \frac{1}{A} J_0(k|\vec{r}_i - \vec{r}_j|) + \frac{1}{A} \text{Im} \sum_{\gamma_{i,j}} \int_{\partial\Omega(\gamma_{i,j})} H_0(k|\vec{r}_i - \vec{r}(s)|) \frac{\partial}{\partial n(s)} H_0(k|\vec{r}(s) - \vec{r}_j|) ds, \quad (3.10)$$

where  $s$  parameterizes a small segment around the bouncing point of the  $\gamma_{i,j}$ -th classical trajectory joining  $\vec{r}_i$  with  $\vec{r}_j$  after just one reflection, and  $n(s)$  is the normal at point  $\vec{r}(s)$ . We mention that uniform approximations can be done in order to render this expression into the usual semiclassical structure sum over paths of some classical prefactor times cosine of some action, but for our purposes this is not necessary.

In figure (3.1) we present our findings for the two-point correlation function  $R^{sc+dif}(\vec{r}_1, \vec{r}_2)$ . Since this is a function of four variables, we present our results by keeping  $\vec{r}_1$  fix, while moving  $\vec{r}_2$  along the line indicated in the insets. The symbols are the exact numerical results, the dashed lines are the predictions of the isotropic contribution to the correlation function coming from the direct classical path (giving both the isotropic Random Wave and Nonlinear Sigma Model results). The continuous line is the sum of the isotropic and first non-isotropic contribution, the later calculated as a sum over all paths with one bounce including diffraction effects.

The comparison with the universal Bessel correlation shows how system dependent effects are essential, particularly close to the boundaries. This is to be expected since the isotropic result obviously misses any non-universal effects. On the other hand, the robustness of the Bessel result is indeed remarkable. We note that the non-zero curvature of the boundary makes the application of the non-isotropic Random Wave Models impossible.

The most spectacular evidence of non-universal effects beyond the Random Wave and Nonlinear Sigma Models is the behavior of the average intensity  $R(\vec{r}, \vec{r})$ . The universal prediction in this approaches gives a constant value  $1/A$  with  $A = \pi$  in our case, while the semiclassical plus diffraction theory predicts a much richer structure.

The results for the average intensity are presented in figure (3.2) for the position  $\vec{r}$  moving along the directions indicated in the inset. The horizontal line without structure is the isotropic result (which is the prediction of the isotropic Random Wave and the Sigma Models), the symbols are the exact quantum mechanical calculations and the continuous line the semiclassical prediction using Eq. (3.10) including diffraction effects.

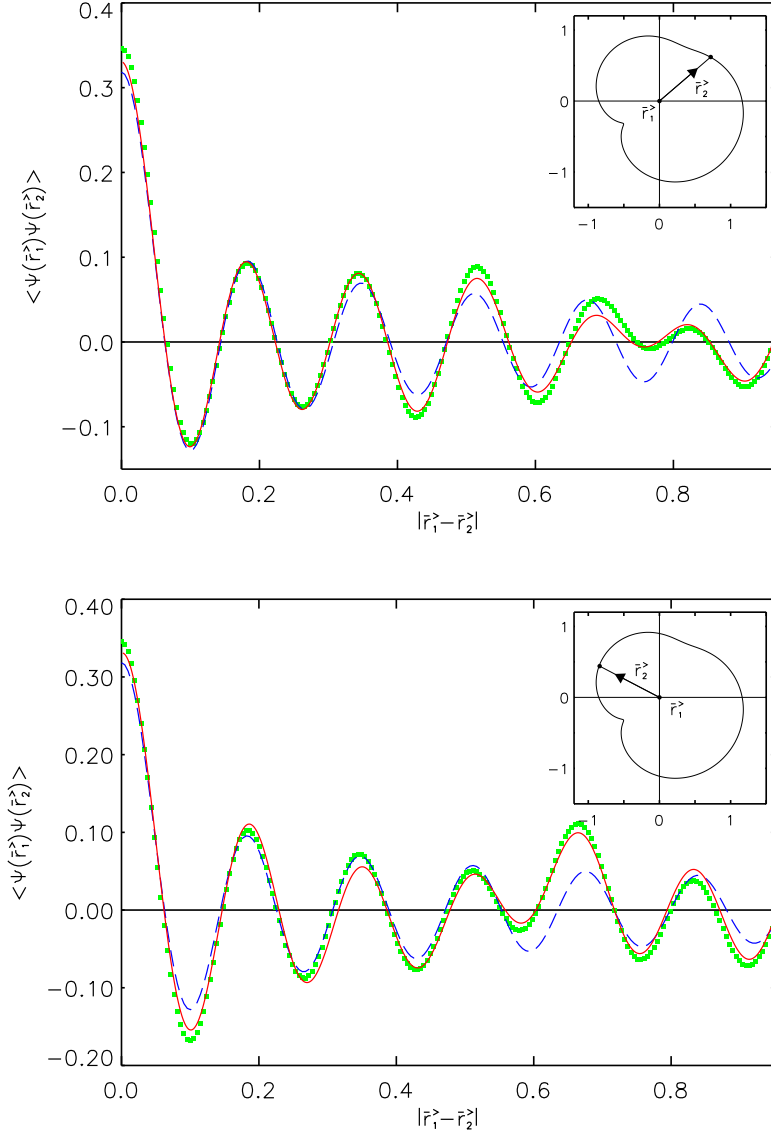


Figure 3.1: Two-point correlation function  $R(\vec{r}_1, \vec{r}_2)$  for  $\vec{r}_2$  pointing along the lines indicated in the Africa billiard (inset). The symbols mark numerical quantum results for  $R$ , Eq. (3.1), the thin lines depict the prediction employing Eq. (3.10) where the Green function is approximated by a sum over paths, including diffraction effects, with at most one reflection at the boundary. The dashed lines shows the result from the isotropic Random Wave and Nonlinear Sigma Model (3.9).

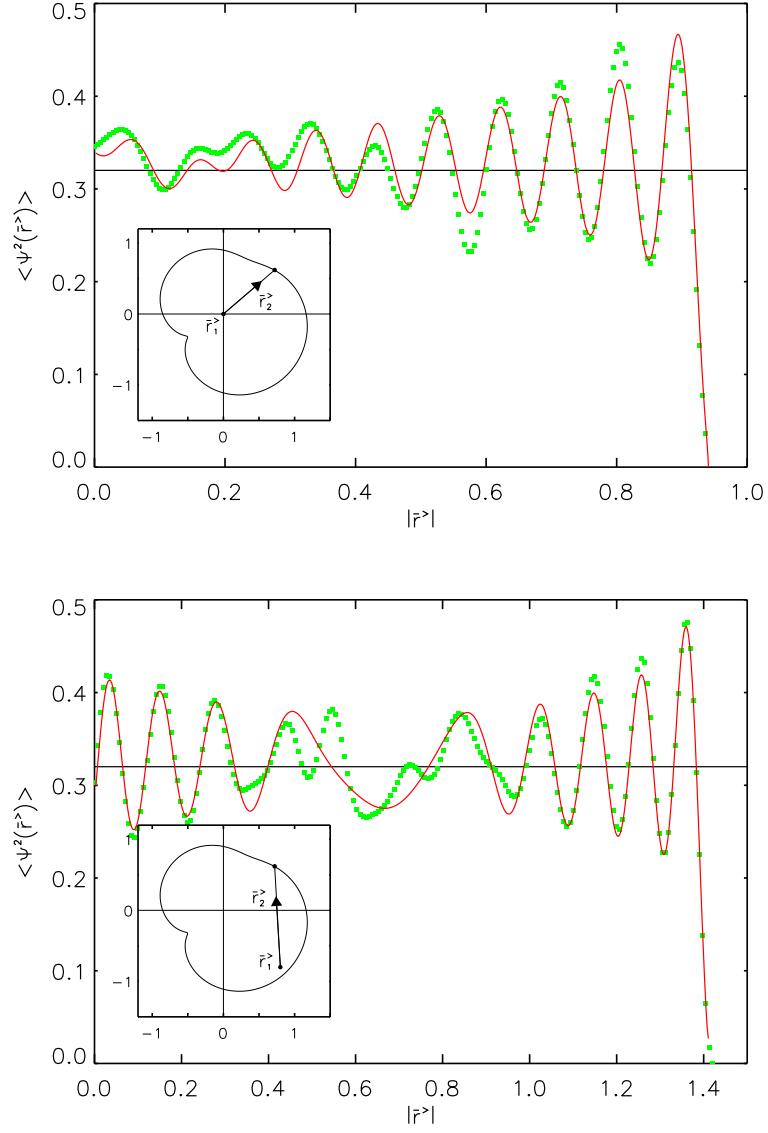


Figure 3.2: Average intensity  $R(\vec{r}, \vec{r})$  for  $\vec{r}$  pointing along the lines indicated in the Africa billiard (inset). The symbols mark numerical quantum results for  $R(\vec{r}, \vec{r})$ , Eq. (3.1), the thin lines depict the prediction employing Eq. (3.10) where the Green function is approximated by a sum over paths, including diffraction effects, with at most one reflection at the boundary. The horizontal line shows the isotropic Random Wave and Nonlinear Sigma Model results ( $1/\pi$ ).

Even when the agreement is not perfect our results clearly indicate the importance of the non-universal effects beyond the isotropic predictions, which are very well described by the semiclassical approach.

On the other hand, since we have systematically used the Gutzwiller version of the semiclassical Green function, and we know this object has serious problems of analyticity, we expect that some effects are not correctly taken into account by the semiclassical two-point correlation presented here, even when supplemented with diffraction effects. This is indeed the case as we discuss now.

## 3.2 Limitations of the semiclassical approach

As we have seen, the semiclassical approach provides a very efficient and appealing way to calculate both universal and non-universal contributions to the quantum two-point correlation function. In principle, the semiclassical approximation has incorporated quantum interference effects in the oscillatory character of the expressions like  $\cos\left(\frac{S}{\hbar}\right)$ . However, as mentioned in the section 1.3, the use of the Gutzwiller Green function comes with non-trivial problems, in particular the destruction of the analytical properties known to characterize its exact quantum mechanical counterpart. Since there is no clear idea about which kind of quantum effects are missing because the lacking of the correct analytical structure of the Green function, the first step in order to study this problem is to construct such meromorphic expression for its semiclassical approximation. This is the major step taken by Fredholm theory.

Once a semiclassical Green function with the correct analytical properties is constructed, one can compare its predictions with the ones coming from the Gutzwiller approach and establish which effects are not correctly incorporated by the second. Due to the complex structure of the Fredholm theory and the huge amount of classical information required to construct the Fredholm Green function, this program has been undertaken only for one very abstract system, but the results are available.

The most notable effects lying beyond the usual semiclassical approach are Anderson localization [42] and scars [55]. Anderson localization is the exponential localization of the wavefunctions in disordered systems and has been an active topic of research for more than 40 years. Since we are dealing here with clean systems, we just mention that the adequate modification of

the semiclassical (Gutzwiller) Green function for disordered systems exists but turns out to be incapable to explain such effect, while presently it is not known how to incorporate disorder effects into the Fredholm approach.

The scar phenomenon, much more relevant for us since it appears in clean systems, was observed for the first time by Heller [55] and consists in the enhancement of the wavefunction intensity in the neighborhood of classical periodic orbits. The importance of this effect for transport and statistical measurements is obvious. Quite an effort has been put on to provide a semiclassical theory of scarring [56], but the only microscopic theory so far able to correctly predict the location and intensity of scars is the Fredholm approach. We can safely conclude that *the statistical theory of eigenfunctions in clean classically chaotic systems based on the Gutzwiller Green function can not correctly incorporate scarring effects due to the incorrect analytical structure of the semiclassical propagator*. Of course, phenomenological recipes can be used to include scarring effects without microscopic derivation “on top” of the results obtained using Gutzwiller theory, but we will not follow such line here.

In any case, the quantum ergodicity theorem demands that the relative density of “scarred” eigenfunctions compared with the whole set of solutions of the Schrödinger equation must converge to zero in the semiclassical limit. This means that in general scarring is an exceptional phenomenon in the statistical sense and then the presence of scarred eigenfunctions will affect only the tails of the probability distributions derived by any statistical theory of eigenfunctions. Some attempts to calculate such effects, clearly non-universal since scarring is strongly system-dependent, have been taken in [56].

The theoretical and numerical results of this section, together with the experimental evidence discussed and the fact that scarring is a statistically small effect give full support to the use of the semiclassical two point correlation function as a building block of a statistical theory of eigenfunctions. The other ingredient must provide the means to go beyond the two-point case and construct any statistical measure of interest, and it is the subject of the next chapter.

## Chapter 4

# The local Gaussian conjecture: Support and implications

As shown in the last chapter, the semiclassical two-point correlation function successfully describes the simplest spatial statistics as the two-point correlation and the average intensity as long as scarring effects can be safely neglected (which is usually the case).

Despite this success, it is obvious that a full statistical description goes far beyond what we can do with just the two-point correlation function. For example, an natural and very pertinent question is: what is the distribution of wavefunction's intensities  $I_1(w, \vec{r})$ , defined as

$$I_1(w, \vec{r}) = \frac{1}{N_W} \sum_{E_l \in W} \delta(w - \psi_l(\vec{r})^2) \quad (4.1)$$

which requires the knowledge of correlation functions of order higher than two?

In this chapter we present the formal statement, the supporting arguments, and the numerical and experimental evidence supporting the *local Gaussian conjecture*, a physically motivated assumption which will allow us to deal with arbitrary statistical measures using only the information encoded in the two-point correlation function.



## 4.1 Mathematical formulation of the local Gaussian conjecture and theoretical support

As usual we consider a 2D closed system with time reversal invariant symmetry. The generalization to arbitrary dimensions and systems with broken time reversal symmetry is straightforward.

Consider the fluctuating quantity  $F_l(\vec{r}_1, \dots, \vec{r}_n) = F(\psi_l(\vec{r}_1), \dots, \psi_l(\vec{r}_n))$  depending on the values of the eigenfunctions at a given set of  $n \ll N_W$  positions. Its exact spectral average  $\mathcal{F}(\vec{r}_1, \dots, \vec{r}_n)$  is given by

$$\mathcal{F}(\vec{r}_1, \dots, \vec{r}_n) = \frac{1}{N_W} \sum_{E_l \in W} F_l(\vec{r}_1, \dots, \vec{r}_n). \quad (4.2)$$

The local Gaussian conjecture consists in considering the set of vectors  $\vec{v}_l = (\psi_l(\vec{r}_1), \dots, \psi_l(\vec{r}_n))$  for  $l = 1, \dots, N_W$  as realizations of a Gaussian  $n$ -dimensional ensemble with distribution

$$P(\vec{v}) = \frac{1}{(2\pi)^{l/2} \sqrt{\det \mathbf{R}}} \exp \left[ -\frac{1}{2} \vec{v} \cdot \mathbf{R}^{-1} \vec{v} \right]. \quad (4.3)$$

This random field is uniquely characterized by the position-dependent  $n \times n$  symmetric *correlation matrix*  $\mathbf{R} = \mathbf{R}(\vec{r}_1, \dots, \vec{r}_l)$  with matrix elements  $R_{i,j} = R(\vec{r}_i, \vec{r}_j)$ . Once the correlation matrix is constructed, all possible averages can be expressed in terms of it by means of Gaussian integration, namely,

$$\mathcal{F}^G(\vec{r}_1, \dots, \vec{r}_n) = \int F(\vec{v}) P(\vec{v}) d\vec{v}. \quad (4.4)$$

The local Gaussian conjecture is then equivalent to assume  $\mathcal{F} = \mathcal{F}^G$ . In other words, *the local Gaussian conjecture claims that the exact eigenfunctions in classically chaotic systems behave like Gaussian random fields uniquely characterized by the exact position-dependent two point correlation function.* We stress that the averages over energy are local in space and depend as indicated on the set of positions which act as parameters of the distribution. For simplicity we suppress the explicit dependence from now on. The main implication of this conjecture is that *all possible statistical averages are given in terms of, and only of, combinations of two-point correlation functions.*

After we have formalized the conjecture, we must consider the physical arguments supporting the affirmation “in a classically chaotic quantum system an ensemble of eigenfunctions with eigenenergies inside an small energy window behave as realizations of a Gaussian random field”.

### 4.1.1 Berry's argument: a critical view

For both conceptual and historical reasons the first argument to consider is the one presented by Berry in his classic paper of 1977 [20] on the spatial structure of regular and irregular wavefunctions.

Berry's idea is to consider the general form of the semiclassical Green function as a sum over classical paths and to fix one on the arguments. The resulting expression, when evaluated at the eigenenergy, is in principle proportional to the corresponding eigenfunction, and is then expressed as a sum of oscillating contributions, one for each path starting at some reference point  $\vec{r}_0$  and ending at the observation position  $\vec{r}$ ,

$$\psi_l(\vec{r}) \sim \sum_{\gamma} A_{\gamma}(\vec{r}, \vec{r}_0) e^{\frac{i}{\hbar} S_{\gamma}(\vec{r}, \vec{r}_0)}. \quad (4.5)$$

Now, it is a well known mathematical fact that the number of classical trajectories joining two given points at fixed energy in a chaotic system increases exponentially with the length [53]. Berry then invokes the central limit theorem to conclude that at least in classically chaotic systems where the intrinsic complexity of the dynamics makes the actions to fluctuate strongly with the energy, the value of the wavefunction at a given point, being given as a large superposition of oscillating uncorrelated terms, will be Gaussian distributed.

The same argument, in one or another form, has been presented to justify statistical treatments in many circumstances, see for example [57], but one must keep in mind that the validity of this result depends strongly in certain assumptions about the wavefunction and the statistical behavior of the semiclassical contributions to it. In particular, to date we don't have any strict proof, neither a very convincing numerical study, supporting the application of the central limit theorem, particularly when we know that the actions must be correlated in order to the eigenfunctions to satisfy the Schrödinger equation and to be normalized.

To put it in few words, the different contributions to the semiclassical wavefunction are indeed correlated, while Berry's argument requires such contributions to be statistically independent.

### 4.1.2 The theoretical-information approach: a critical review

Following a very different approach, Srednicky and coworkers [46] also argue the Gaussian assumption by means of an information-theoretical approach known as Principle of Maximum Entropy (PME).

The PME has a notable history, starting by the works of Gibbs in the mechanical foundations of statistical physics, but it was Jaynes who developed it to a very sophisticated and powerful tool to construct statistical distributions in general situations (for an excellent presentation see [58]).

The PME starts defining a functional of the probability distribution called entropy, and then postulates that the correct distribution is such that the entropy is maximized under the possible constraints imposed on the distribution, usually in the form of expected values.

In the case of chaotic wavefunctions we have two kinds of constrictions. On one side we demand the eigenfunctions to solve the Schrödinger equation, with the appropriate boundary conditions, and/or to be normalized. Since such requirements fully determine the eigenfunction, it is quite obvious that for statistical purposes we are asking too much.

The easiest thing is then to use the only information we have at hand, namely, the semiclassical two-point correlation function. Since this is a bilinear quantity in the wave function, the resulting distribution is the only distribution fully determined by the two-point averages, namely, a Gaussian field.

The reason why this argument can not be considered as a full proof of the Gaussian conjecture but just a method to optimize the information encoded in the two-point correlation function is twofold. On one side it excludes all the effects of the correct normalization of the eigenfunctions. Such effects are indeed difficult to incorporate in any PME, despite the claims made in [57], simply because the exact normalization can not be cast in the form of an average. Second, the probability to find a given state for a given physical system must be a characteristic of the state itself, not of our partial knowledge about the system as expressed by the PME.

### 4.1.3 The quantum ergodicity argument: a critical review

In our opinion, the most appealing and mathematically sound argument towards the Gaussian conjecture is based in quantum ergodicity [59].

The idea is to use the scattering approach to quantization [60], in which the exact eigenfunctions are written as linear combinations of basis functions with certain coefficients. Such coefficients are the components of the eigenvectors of the scattering matrix. Quantum ergodicity ensures that for classically chaotic systems the eigenvectors of the  $S$  matrix are only restricted to be normalized and it is easily proven that this implies a Gaussian distribution for their components in the high energy limit. Using this property, it can be shown that the eigenfunctions behave as Gaussian random fields.

As with the others arguments, the quantum ergodicity idea faces problems with the normalization condition, which turns out again very difficult to incorporate. There is, however, another conceptual difficulty: the eigenvectors of the  $S$  matrix corresponding to eigenfunctions of the Hamiltonian are rather special (they correspond to the unit eigenvalue of the  $S$  matrix) and then it is difficult to justify the use of ergodic arguments based in the “genericity” of the eigenvectors involved.

## 4.2 Relation with Random Matrix Theory

We know that the Random Matrix Theory provides results not only for the statistics of eigenvalues, but for the statistical properties of eigenfunctions, some of them checked with a high degree of accuracy, so a word about the relation between the Gaussian conjecture and the RMT is in order.

Strictly speaking, the Random Matrix Theory predicts that eigenfunctions have fully uncorrelated components with Gaussian distribution [26], and is the limit  $\tilde{R} = 0$  of the local Gaussian theory. The claim, frequently heard, that Berry’s ansatz is equivalent the Random Matrix Theory must be taken cautiously.

The Gaussian conjecture comes from a pure semiclassical context and it is conceptually independent of the Random Matrix Theory. To put it in more dramatic terms, the essential property of the RMT ensembles is their invariance under changes of basis in Hilbert space, and this invariance is broken when the different values of the eigenfunctions are correlated. *The*

*results of the isotropic Random Wave Model can not be derived within the Random Matrix Theory and its conceptual foundations are fully independent.* Since we know that the isotropic Random Wave Model is a Gaussian field where the universal limit of the two-point correlation function is used, we see that already in the universal regime there are results coming from the semiclassical theory beyond the Random Matrix Theory.

In order to extend the Random Matrix Theory beyond the case of uncorrelated values of the wavefunction we must use the Sigma Models, since they correctly incorporate the isotropic Random Wave Model as their universal limit.

### 4.3 Numerical check of the local Gaussian conjecture

All numerical (see for example [52, 60, 61]) and experimental (see for example [62]) evidence accumulated the last years show the impressive predictive power of the Random Wave Model. As we explained, this is a direct consequence of the robustness of the Bessel-like correlation function when spatial averages are involved.

A direct test of the local version of the Gaussian conjecture is a very demanding numerical or experimental task. The reason is that without the extra spatial average the number of samples is dramatically reduced. This, together with the restriction imposed on the energy window made it impossible so far to check any non-trivial local statistical measure in billiard systems, like the local distribution of intensities. The local two-point correlation beyond the isotropic regime has been tested in [40] in the context of the non-isotropic Random Wave Model. Since, as we will show in chapter VI, this is a particular case of the semiclassical approach, such numerical check also gives support to our ideas.

We can argue, however, that as long as localization effects can be neglected, any chaotic system should be good enough to test the validity of the local Gaussian conjecture. This give us the freedom to work with a particular kind of systems with better statistical properties, namely, where the amount of available data is far larger than in Hamiltonian systems. We have tested the conjecture for a quantum map [49] using the raw data presented in [63] for the discrete-time time evolution operator for a system periodically kicked.

The advantage of this kind of systems is that all the eigenfunctions have similar statistical properties and the restriction about the energy window is not relevant anymore, for details see [63].

To perform a numerical test of the local Gaussian conjecture, we used the numerically exact quantum mechanical data of [63] and calculate the integrated distribution of intensities

$$P(w) = \int I_1(w, \vec{r}) d\vec{r} \quad (4.6)$$

exactly. The global Gaussian conjecture, namely, a Gaussian field with diagonal correlation matrix independent of the position gives the well known Porter-Thomas result from Random Matrix Theory,

$$P^{RMT}(w) = \frac{A^{1/2}}{(2\pi w)^{1/2}} e^{-\frac{Aw}{2}} \quad (4.7)$$

while the prediction of the local Gaussian theory is

$$P^G(w) = \int \frac{1}{\sqrt{2\pi w R(\vec{r}, \vec{r})}} \exp\left(-\frac{w}{2R(\vec{r}, \vec{r})}\right) d\vec{r}. \quad (4.8)$$

In order to check the local Gaussian conjecture we proceed like this:

- we use the exact numerical results to numerically construct the local average intensity  $R(\vec{r}, \vec{r})$ , and
- we numerically integrate the local intensity distribution over the space to obtain  $P^G(w)$ .

Our results are summarized in figure (4.1). The symbols are the exact quantum mechanical distribution constructed using the definition,  $P(w)$ . The dashed line is the RMT result,  $P^{RMT}(w)$  and the solid line is the integrated local Gaussian result obtained with the exact quantum mechanical average intensity,  $P^G(w)$ .

We note that the exact calculations deviate from the RMT prediction both in the bulk (inset) and the tails of the distribution, while the local Gaussian theory is in perfect agreement with the exact numerical results. This most demanding test specifically dedicated to the local Gaussian conjecture indicates its validity, and shows the way to calculate non-universal

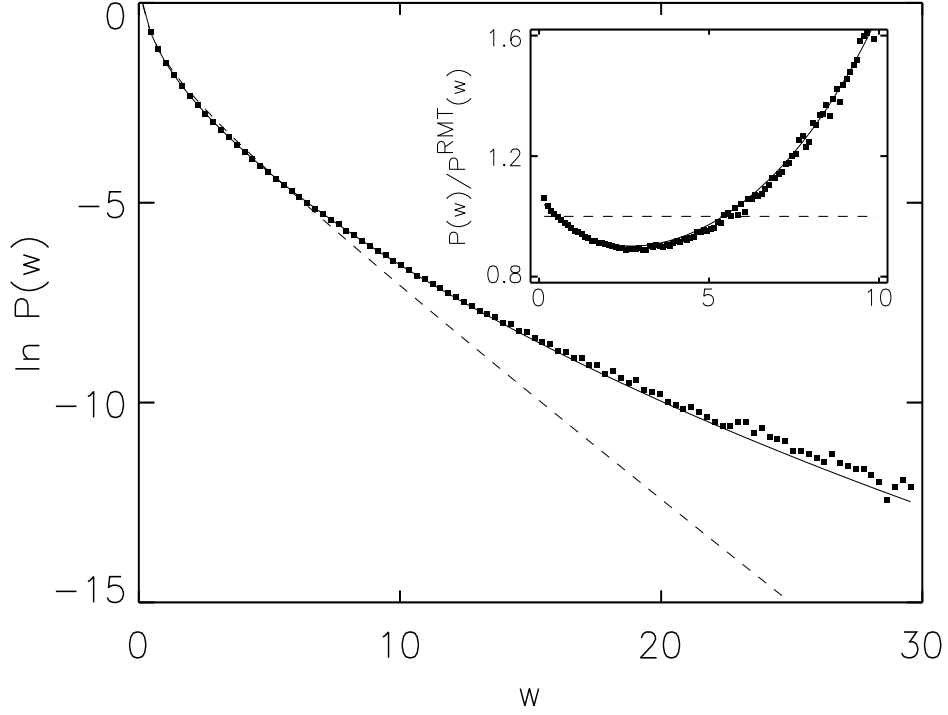


Figure 4.1: Integrated distribution of intensities  $P(w) = \int I_1(w, \vec{r}) d\vec{r}$  for the a quantum kicked system in the chaotic regime. The inset shows the bulk of the distribution, the big figure includes the tails. The symbols are the quantum mechanical exact numerical calculations (based on raw data from [63]), using the definition of  $I(w, \vec{r})$  and numerical integration. The dashed line is the RMT result  $P^{RMT}(w) = \frac{A^{1/2}}{(2\pi w)^{1/2}} e^{-w(A/2)}$  and the solid line the result obtained by using the local Gaussian conjecture for  $I_1^G(w, \vec{r})$  fixed by the average intensity  $R(\vec{r}, \vec{r})$  calculated exactly form the numerical results.

effects beyond Random Matrix Theory: *non-universal effects are related with the spatial fluctuations of the local correlation matrix.*

In the next chapter we present the structure of the full theory based on the local Gaussian conjecture and the semiclassical two-point correlation function.



## Chapter 5

# The Gaussian theory of eigenfunctions: formal structure and semiclassical approximation

In this chapter we put together the semiclassical correlation function and the Gaussian conjecture, and show how to operate with the theory that results. Although manifestly similar approaches have been used in a number of situations [57, 64, 65], we are not aware of the use of this hybrid technique beyond the universal (Random Wave Model) predictions. We present here the first systematic use of this theory to go beyond the Random Wave and the Sigma Models.

The ingredients missed in previous works are:

- the explicit use of the energy average, which implies the existence of a cut-off time in the periods of the classical trajectories involved,
- the consistent semiclassical expansion, which takes into account the scaling with  $\hbar_{eff}$  of the contributions beyond Random Matrix Theory, and
- the separation of the results in their “oscillatory” and “non-oscillatory” contributions, which reveals the classical backbone of the results.

In this chapter we introduce the basic mathematical method to deal with Gaussian integrals (Wick’s theorem), then we continue the program by ex-

panding the general expression for any average up to the second semiclassical order, and finally we explain which are the oscillatory and non-oscillatory contributions to the general result.

## 5.1 Gaussian integrals

As shown in the past chapter, the average of any statistical measure is, using the Gaussian conjecture, boiled down to the calculation of Gaussian integrals over  $n$ -dimensional vectors, where  $n$  is the order of the statistics (the number of different positions at which the wavefunction is required). From now on  $\langle \dots \rangle$  will indicate average over the multi-dimensional Gaussian distribution  $P(\vec{v})$  given by

$$P(\vec{v}) = \frac{1}{(2\pi)^{n/2} \sqrt{\det \mathbf{R}}} \exp \left[ -\frac{1}{2} \vec{v} \cdot \mathbf{R}^{-1} \vec{v} \right], \quad (5.1)$$

with  $\mathbf{R}$  the (positive definite) correlation matrix, which depends parametrically on the spatial points where the statistics are considered through its matrix elements  $R_{i,j} = R(\vec{r}_i, \vec{r}_j)$  given in terms of the correlation function.

The most general and important result concerning Gaussian integrals in high dimensional spaces is Wick's theorem, which states that,

$$\begin{aligned} \left\langle \prod_{i=1}^{2n} v_i \right\rangle &= \sum_{\sigma=1}^{(2n-1)!!} \prod_{q=1}^n R_{\sigma_q}, \\ \left\langle \prod_{i=1}^{2m+1} v_i \right\rangle &= 0, \end{aligned} \quad (5.2)$$

where  $\sigma_q$  is the  $q$ -th pair of the  $\sigma$ -th contraction, the later given by one of the  $(2n-1)!!$  pairwise combination of the indexes  $1, \dots, 2n$ . The proof of this theorem can be found in any standard book of statistics (for example [68]). Note that, as expected,

$$\langle v_i v_j \rangle = R_{i,j}. \quad (5.3)$$

Another very useful (and equivalent) version of Wick's theorem allows us to quickly calculate the characteristic function of the Gaussian distribution:

$$\langle e^{i\vec{u} \cdot \vec{v}} \rangle = \exp \left[ -\frac{1}{2} \vec{u} \cdot \mathbf{R} \vec{u} \right]. \quad (5.4)$$

Wick's theorem provides a straightforward connection between any kind of average and the only input of the theory, namely the correlation matrix expressed in terms of the two-point correlation function.

### 5.1.1 Some examples: relating non trivial statistics with the two-point correlation function

Once the Gaussian average is performed, any statistical measure will be expressed in terms of all possible correlation functions  $R(\vec{r}_i, \vec{r}_j)$  constructed by joining all possible pair of positions involved. At this point we have not made any use of the semiclassical approximation and the results rely only on the Gaussian conjecture.

The full semiclassical theory appears when instead of the exact  $R(\vec{r}_i, \vec{r}_j)$  we use its semiclassical approximation

$$R^{sc}(\vec{r}_i, \vec{r}_j) = \frac{1}{A(e)} \left( \delta_{i,j} + \tilde{R}(\vec{r}_i, \vec{r}_j) \right) \quad (5.5)$$

with

$$\tilde{R}(\vec{r}_i, \vec{r}_j) = \sum_{\gamma_{i,j}} \Gamma \left( \frac{T_{\gamma_{i,j}}}{\tau_W} \right) \left| \frac{2\hbar}{\pi m^2} D_{\gamma_{i,j}} \right|^{1/2} \cos \left( \frac{S_{\gamma_{i,j}}}{\hbar} \right), \quad (5.6)$$

to obtain any statistical measure in terms of sums over classical paths with periods up to the cut-off time  $\tau_W = \hbar/\delta e$  depending on the size of the energy window.

We start with the simplest case, the calculation of the wavefunction's moments at a given point  $\langle \psi(\vec{r})^n \rangle$ . This measure is expressed in terms of the  $n$ -th point correlation function as:

$$\begin{aligned} \langle \psi(\vec{r})^n \rangle &= R_n(\vec{r}_1 = \vec{r}, \dots, \vec{r}_n = \vec{r}) \\ &= \frac{1}{N_W} \sum_{E_l \in W} \psi_l(\vec{r})^n, \end{aligned} \quad (5.7)$$

where the last line expresses the Gaussian conjecture. This are one-point statistics involving a single degree of freedom (the value of the wavefunction at point  $\vec{r}$ ). In our notation the vector  $\vec{v}$  has just one component  $v = \psi(\vec{r})$  and the only entry of the correlation matrix takes the form:

$$R_{1,1} = \langle \psi(\vec{r}) \psi(\vec{r}) \rangle = R(\vec{r}, \vec{r}). \quad (5.8)$$

Gaussian integration gives  $\langle v^{2n+1} \rangle = 0$  and

$$\langle v^{2n} \rangle = (2n-1)!! R_{1,1}^n. \quad (5.9)$$

Finally, use of the semiclassical correlation function Eq. (5.6), leads to an expression in terms of classical paths:

$$\langle \psi(\vec{r})^{2n} \rangle = \frac{(2n-1)!!}{A(e)^n} \left[ 1 + \tilde{R}(\vec{r}, \vec{r}) \right]^n. \quad (5.10)$$

Observe the intuitive structure of the result in the semiclassical picture: the moments of the intensity are related with classical paths starting and ending at the observation point.

Now we can calculate the full distribution of intensities at a given point. This is an important measure which has been carefully analyzed [66,67] and was numerically studied in the last chapter. It is defined as

$$\begin{aligned} \langle \delta(w - \psi(\vec{r})^2) \rangle &= I_1(w, \vec{r}) \\ &= \frac{1}{N_W} \sum_{E_l \in W} \delta(w - \psi_l(\vec{r})^2), \end{aligned} \quad (5.11)$$

and again the last equality assumes the Gaussian conjecture. This is also a one-point statistic and the corresponding Gaussian integral is then simply:

$$\langle \delta(w - v^2) \rangle = \frac{1}{\sqrt{2\pi R_{1,1}}} \exp \left[ -\frac{w}{2R_{1,1}} \right], \quad (5.12)$$

which then gives the local distribution

$$\langle \delta(w - \psi(\vec{r})^2) \rangle = \sqrt{\frac{A(e)}{2\pi(1 + \tilde{R}(\vec{r}, \vec{r}))}} \exp \left[ -\frac{A(e)w}{2(1 + \tilde{R}(\vec{r}, \vec{r}))} \right], \quad (5.13)$$

in terms of the sum over classical paths  $\tilde{R}(\vec{r}, \vec{r})$ . This is the local generalization of the Porter-Thomas distribution [26], given by  $\tilde{R}(\vec{r}, \vec{r}) = 0$ .

Let us consider now two-point statistics. One very well studied example is the two-point correlation of the intensity. It is defined in terms of the general correlation function as

$$\begin{aligned} \langle \psi(\vec{r}_1)^2 \psi(\vec{r}_2)^2 \rangle &= R_4(\vec{r}_1, \vec{r}_1, \vec{r}_2, \vec{r}_2) \\ &= \frac{1}{N_W} \sum_{E_l \in W} \psi_l(\vec{r}_1)^2 \psi_l(\vec{r}_2)^2. \end{aligned} \quad (5.14)$$

In this case  $\vec{v}$  has two components

$$(v_1, v_2) = (\psi(\vec{r}_1), \psi(\vec{r}_2)), \quad (5.15)$$

and the correlation matrix is a two by two matrix. The Gaussian average is done using Wick's theorem to get

$$\langle v_1^2 v_2^2 \rangle = R_{1,1} R_{2,2} + 2R_{1,2}^2, \quad (5.16)$$

and in terms of classical paths

$$\begin{aligned} \langle \psi(\vec{r}_1)^2 \psi(\vec{r}_2)^2 \rangle &= \frac{1}{A(e)^2} (1 + \tilde{R}(\vec{r}_1, \vec{r}_1))(1 + \tilde{R}(\vec{r}_2, \vec{r}_2)) \\ &+ \frac{2}{A(e)^2} \tilde{R}(\vec{r}_1, \vec{r}_2)^2. \end{aligned} \quad (5.17)$$

We note again a very intuitive structure when the result is seen in semiclassical terms: the intensity-intensity correlation function contains contributions from classical closed paths passing through  $\vec{r}_1$ , classical closed paths passing through  $\vec{r}_2$  and classical open paths joining  $\vec{r}_1$  with  $\vec{r}_2$ .

## 5.2 The consistent semiclassical expansion and the general structure of the averages

After the last examples we see that the Gaussian conjecture, together with the semiclassical correlation function, can be used to provide closed results for statistical measures, but it is also clear that the more complicated the measure, the more involved the expressions. There is, however, a further consideration that, without using any new approximation, drastically simplify the results:

- the semiclassical approach, expressing the results as complicated functions of  $\tilde{R} \sim \hbar_{eff}^{1/2}$  cannot correctly incorporate any contribution of higher order than  $\tilde{R}^2 \sim \hbar_{eff}$ , since the semiclassical expression for the correlation function already neglects terms of order  $\hbar_{eff}^{3/2}$ .

The practical implication of this observation is that *the results of the semiclassical theory are meaningful only up to second semiclassical order around  $\tilde{R} = 0$* . This observation lies at the heart of our work: it means that the

completely general structure of any  $n$ -point statistical measure  $\mathcal{F}(\vec{r}_1, \dots, \vec{r}_n)$  within the semiclassical approach has the form

$$\begin{aligned} \mathcal{F} = \mathcal{F}^{RMT} &+ \frac{1}{2} \sum_{i,j}^n \mathcal{F}^{i,j} \tilde{R}_{i,j} - \frac{1}{2} \sum_{i,j,k}^n \mathcal{F}^{i,j,k} \tilde{R}_{i,k} \tilde{R}_{k,j} \\ &+ \frac{1}{8} \sum_{i,j,k,o}^n \mathcal{F}^{i,j,k,o} \tilde{R}_{i,j} \tilde{R}_{k,o}, \end{aligned} \quad (5.18)$$

in terms of single and double sums over classical trajectories (the numerical factors are chosen to simplify further results).

This analysis has another fundamental consequence. Since the consistent semiclassical expansion is taken around  $\tilde{R} = 0$ , and all system-specific features are included only in  $\tilde{R}$ , *the coefficients  $\mathcal{F}^{RMT}$ ,  $\mathcal{F}^{i,j}$ ,  $\mathcal{F}^{i,j,k}$  and  $\mathcal{F}^{i,j,k,l}$  are universal functions, independent of the particular system* (in particular,  $\mathcal{F}^{RMT}$  is the Random Matrix Theory average). We proceed now to the evaluation of this universal coefficients.

### 5.2.1 Calculation of the universal coefficients

For a specific problem, in principle, the universal coefficients are calculated by solving the Gaussian integrals and then expanding the results in terms of all possible combinations  $\tilde{R}(\vec{r}_i, \vec{r}_j)$  up to second order.

There is, however, a more general way to approach the problem, namely, by direct expansion of the Gaussian distribution in powers of  $\tilde{R}(\vec{r}_i, \vec{r}_j)$ , so we do not need to make different calculations for different measures.

First, we write the correlation matrix as  $\mathbf{R} = A(e)^{-1}(\mathbf{I} + \tilde{\mathbf{R}})$  with  $\mathbf{I}$  the  $n \times n$  unit matrix and factorize out the Random Matrix Theory distribution (which corresponds to  $\tilde{\mathbf{R}} = 0$ ) from the local Gaussian distribution,

$$\begin{aligned} \frac{\exp \left[ -\frac{1}{2} \vec{v} \cdot \mathbf{R}^{-1} \vec{v} \right]}{(2\pi)^{n/2} \sqrt{\det \mathbf{R}}} &= \left( \frac{A(e)}{2\pi} \right)^{n/2} \frac{\exp \left[ -\frac{A(e)}{2} \vec{v} \cdot (\mathbf{I} + \tilde{\mathbf{R}})^{-1} \vec{v} \right]}{\sqrt{\det(\mathbf{I} + \tilde{\mathbf{R}})}} \\ &= \left( \frac{A(e)}{2\pi} \right)^{n/2} \exp \left[ -\frac{A(e)}{2} \vec{v} \cdot \vec{v} \right] \tilde{P}(\vec{v}; \tilde{\mathbf{R}}) \\ &= P^{RMT}(\vec{v}) \tilde{P}(\vec{v}; \tilde{\mathbf{R}}). \end{aligned} \quad (5.19)$$

All the effects beyond Random Matrix Theory are included into the distribution

$$\tilde{P}(\vec{v}; \tilde{\mathbf{R}}) = \frac{1}{\sqrt{\det(\mathbf{I} + \tilde{\mathbf{R}})}} \exp \left[ \frac{A(e)}{2} \vec{v} \cdot \frac{\tilde{\mathbf{R}}}{\mathbf{I} + \tilde{\mathbf{R}}} \vec{v} \right]. \quad (5.20)$$

Now we can expand  $\tilde{P}(\vec{v}; \tilde{\mathbf{R}})$  up to second order in  $\tilde{\mathbf{R}}$ .

First we need two formal results valid for any bounded matrix  $\epsilon$  and a real number  $\alpha$

$$\begin{aligned} \exp \left[ \alpha \vec{v} \cdot \frac{\epsilon}{\mathbf{I} + \epsilon} \vec{v} \right] &= \exp \left[ \alpha \vec{v} \cdot (\epsilon - \epsilon^2) \vec{v} + O(\epsilon^3) \right] \\ &= 1 + \alpha \vec{v} \cdot \epsilon \vec{v} - \alpha \vec{v} \cdot \epsilon^2 \vec{v} + \frac{\alpha^2}{2} (\vec{v} \cdot \epsilon \vec{v})^2 + O(\epsilon^3), \end{aligned} \quad (5.21)$$

and

$$\begin{aligned} \det(\mathbf{I} - \epsilon)^{-\frac{1}{2}} &= e^{-\frac{1}{2} \text{tr} \log(\mathbf{I} - \epsilon)} \\ &= e^{\frac{1}{2} \text{tr} \left[ \sum_{l=1}^{\infty} \frac{\epsilon^l}{l} \right]} \\ &= e^{\frac{1}{2} \text{tr} \left[ \epsilon + \frac{\epsilon^2}{2} + O(\epsilon^3) \right]} \\ &= 1 + \frac{1}{2} \text{tr} \left[ \epsilon + \frac{\epsilon^2}{2} + O(\epsilon^3) \right] + \frac{1}{8} \left( \text{tr} \left[ \epsilon + \frac{\epsilon^2}{2} + O(\epsilon^3) \right] \right)^2 + O(\epsilon^3) \\ &= 1 + \frac{1}{2} \text{tr} \epsilon + \frac{1}{4} \left[ \text{tr} \epsilon^2 + \frac{1}{2} (\text{tr} \epsilon)^2 \right] + O(\epsilon^3). \end{aligned} \quad (5.22)$$

Using this formal results we can express the local Gaussian distribution as

$$P(\vec{v}) = P^{RMT}(\vec{v}) \left[ 1 + \tilde{P}^{(1)}(\vec{v}) + \tilde{P}^{(2)}(\vec{v}) \right] + O(\tilde{\mathbf{R}}^3), \quad (5.23)$$

with the contributions to first and second semiclassical order given by

$$\tilde{P}^{(1)}(\vec{v}) = \frac{1}{2} \left[ A(e) \vec{v} \cdot \tilde{\mathbf{R}} \vec{v} - \text{tr} \tilde{\mathbf{R}} \right] \quad (5.24)$$

$$\begin{aligned} \tilde{P}^{(2)}(\vec{v}) &= \frac{A(e)(\text{tr} \tilde{\mathbf{R}})}{4} \vec{v} \cdot \tilde{\mathbf{R}} \vec{v} + \frac{1}{4} \left[ \text{tr} \tilde{\mathbf{R}}^2 + \frac{(\text{tr} \tilde{\mathbf{R}})^2}{2} \right] \\ &+ \frac{1}{2} \left[ \frac{A(e)^2 (\vec{v} \cdot \tilde{\mathbf{R}} \vec{v})^2}{4} - A(e) \vec{v} \cdot \tilde{\mathbf{R}}^2 \vec{v} \right]. \end{aligned} \quad (5.25)$$

Now we can explicitly evaluate the average of an arbitrary statistical measure  $F(\vec{v})$  up to second order in  $\tilde{\mathbf{R}}$

$$\begin{aligned}\mathcal{F}(\vec{r}_1, \dots, \vec{r}_n) &= \int F(\vec{v}) P(\vec{v}) d\vec{v} \\ &= \int F(\vec{v}) P^{RMT}(\vec{v}) \left[ 1 + \tilde{P}^{(1)}(\vec{v}) + \tilde{P}^{(2)}(\vec{v}) \right] d\vec{v},\end{aligned}\tag{5.26}$$

and compare with the general expression Eq. (8.1) to obtain the universal coefficients in terms of Random Matrix Theory averages

$$\begin{aligned}\mathcal{F}^{RMT} &= \langle F(\vec{v}) \rangle_{RMT}, \\ \mathcal{F}^{i,j} &= A(e) \langle F(\vec{v}) v_i v_j \rangle_{RMT} - \langle F(\vec{v}) \rangle_{RMT} \delta_{i,j}, \\ \mathcal{F}^{i,j,k} &= A(e) \langle F(\vec{v}) v_i v_j \rangle_{RMT}, \\ \mathcal{F}^{i,j,k,o} &= A(e)^2 \langle F(\vec{v}) v_i v_j v_k v_o \rangle_{RMT} - 2A(e) \langle F(\vec{v}) v_i v_j \rangle_{RMT} \delta_{k,o} \\ &\quad + 3 \langle F(\vec{v}) \rangle_{RMT} \delta_{i,o} \delta_{j,k}\end{aligned}\tag{5.27}$$

Equations (5.6), (5.18) and (5.27) are the general results of our approach. They express the results of any possible average in terms of the universal coefficients (independent of the particular system) and sums over classical trajectories.

We remark that the final step in our approach (expanding the results up to second order in  $\hbar_{eff}$ ) *is not* a further approximation but a consistent application of the semiclassical methods. The whole theory is based on a conjecture (the local Gaussian conjecture) and one unique approximation scheme, the semiclassical approximation.

### 5.2.2 The oscillatory and non-oscillatory contributions

The general result obtained in terms of universal coefficients is just a formal consequence of the Gaussian conjecture and the semiclassical approximation. Another concept which will provide deep insight into the general structure of the semiclassical results is the use of the diagonal approximation (in the spirit of Berry [69]) to separate oscillatory and non-oscillatory contributions.

We mentioned in the introduction that the power of the semiclassical methods lies in the incorporation of interference effects, following the structure of the Feynman propagator in which each path carries a phase and the quantum propagation is the coherent superposition of all possible contributions coming from all possible paths.



Interference effects, we also mentioned, can not be described by finite-order perturbation theory in  $\hbar_{eff}$ , because they contain an essential singularity at  $\hbar_{eff} = 0$ . However, there are quantum corrections to the pure classical results which can be described in terms of (finite) powers of  $\hbar_{eff}$ . Examples are the higher order corrections to the Thomas-Fermi approximation to the density of states [70], or the quantum corrections to the Boltzmann equation founded in the framework of the Wigner-Moyal formalism.

Typically, interference effects produce *oscillatory contributions* (in space, energy, or when an external parameter is varied), and then they are more sensitive to averaging mechanisms than the *non oscillatory contributions* which are typically monotonic functions of position, energy or external parameters. In order to separate the two types of contributions we note that the general structure of our results involves sums and double sums over classical trajectories. The sums over single trajectories are always oscillatory, since each term is proportional to  $\cos(S/\hbar)$ . The only possibility to obtain non-oscillatory contributions is by cancellation of phases in the double sum, namely, by considering pairs of trajectories with similar actions.

Classifying in general the actions of classical trajectories is a very difficult task (see [71]), so we follow Berry [69] assuming that in chaotic systems the actions of classical trajectories with period much shorter than the Heisenberg time are statistically uncorrelated. In practical terms, Berry's diagonal approximation means that the non-oscillatory contribution to the semiclassical results comes only from pairing trajectories with themselves in the double sums. We remark, however, that there are known situations where another type of pairing can lead to non-oscillatory contributions to the semiclassical predictions. These are the so-called "loop" contributions [72, 73], and their incorporation into our approach is presently matter of investigation.

With these remarks in mind, in diagonal approximation the non-oscillatory (n.o) contribution to a general statistical measure is

$$\begin{aligned} \mathcal{F}^{n.o}(\vec{r}_1, \dots, \vec{r}_n) &= \mathcal{F}^{RMT} \\ &+ \frac{\hbar}{8\pi m^2} \sum_{i,j} F^{i,j} \left[ \sum_{\gamma_{i,j}} D_{\gamma_{i,j}} \Gamma^2 \left( \frac{T_{\gamma_{i,j}}}{\tau_W} \right) \right], \end{aligned} \quad (5.28)$$

with

$$F^{i,j} = \mathcal{F}^{i,j,i,j} + \mathcal{F}^{i,j,j,i} - 4\mathcal{F}^{i,i,j} - \delta_{i,j} \mathcal{F}^{i,i,i,i}, \quad (5.29)$$

while the non-oscillatory contribution is then given by  $\mathcal{F}^o(\vec{r}_1, \dots, \vec{r}_n) =$

$$\mathcal{F}(\vec{r}_1, \dots, \vec{r}_n) - \mathcal{F}^{n.o}(\vec{r}_1, \dots, \vec{r}_n).$$

The physical interpretation of the non-oscillatory contributions to the statistics will be discussed in chapter VI but we note that, as promised, it is a monotonic function of both energy and position, and in general it will not be washed out by an extra average. This robustness makes the non-oscillatory contribution extremely important to describe experimental measurements because they typically involve more than one averaging mechanism.

## Chapter 6

# Formal applications of the theory

The statistical theory of eigenfunctions presented in the last chapter has a conceptual problem in common with the other existing approaches (the Random Wave and Ballistic Sigma Models): *it lacks a fully microscopic formal derivation*. However, while one ingredient of the theory is a microscopic and extensively tested approximation method (the semiclassical approximation), the other has considerable theoretical, numerical and experimental support (the Gaussian conjecture).

It is then appealing to consider this approach as close to the fundamental microscopic theory of eigenfunction's statistics (at least for clean classically chaotic systems), but first its connection with the Random Wave and Sigma Models must be clarified.

In order to consider the Gaussian-semiclassical approach as more fundamental, two conditions must be fulfilled:

- We should be able to derive all the available results obtained using the Random Wave and Sigma Model approaches in well defined limits of the Gaussian theory. Such correspondence must be established in the particular physical situation where the Random Wave Model and Ballistic Sigma Model results hold.
- We should provide numerical or experimental evidence showing that the effects predicted by the Gaussian theory which are not present in the other approaches are indeed of physical origin and not a mere artifact of the theory.

A third aspect, not conceptual but practical, concerns the degree of technical manipulations and the complexity of the mathematics leading to specific predictions. However, after we have derived a general formula to calculate any possible statistical measure using the Gaussian approach (something that has not been done using any other theory so far), the practical feasibility of our ideas is beyond doubt, but more evidence in this direction will be presented in this chapter.

In this chapter we will show that:

- The isotropic and non-isotropic Random Wave Models are limiting cases of the Gaussian theory corresponding to particular idealizations of the system's boundaries.
- The available results of the Ballistic Sigma Model concerning the statistical properties of irregular eigenfunctions are limiting cases of the results obtained using the Gaussian theory. This limit correspond to situations where oscillatory contributions can be neglected and a zero-width energy window is taken.

We will also discuss the existing evidence showing that

- effects beyond the Random Wave Models due, in particular, to the non-zero curvature of the boundaries has been observed numerically, and
- the oscillatory contributions beyond the Ballistic Sigma Model have physical origin and have been observed both numerically and experimentally,

to definitively clarify the relationship among the three approaches: Gaussian-semiclassical, and the Random Wave and Sigma Models.

## 6.1 Derivation of the Random Wave Models

The first formal challenge of our approach is to construct the known Random Wave Models by means of the Gaussian conjecture and the semiclassical two-point correlation function instead of using random superpositions of basis functions.

The good news is that any random superposition of basis functions produce Gaussian statistics [74], and then the theory is fully and uniquely specified by its two-point correlation function.

Our problem is then reduced to calculate the two-point correlation functions predicted by the Random Wave Models, for the particular geometries where they are derived, using the expression for the correlation function in terms of the Green function or its semiclassical approximation. This will provide microscopic grounds to one aspect of the models, leaving the Gaussian conjecture as the only assumption.

### 6.1.1 The isotropic Random Wave Model

The isotropic random Wave Model assumes constant potential and neglects any effect due to the boundary. When this is a good approximation, as it is typically the case for the bulk in billiard systems, the exact Green function is well approximated by the Green function of the free particle. In the limit large system area, where this approximation holds better, the mean level spacing approaches to zero (reflecting the infinite degeneracy of the eigenstates of the free particle) and the limit  $\delta e \rightarrow 0$  can be consistently taken.

The result for the two-point correlation function is then Berry's result, as explained in section 3.1.1. *the isotropic Random Wave Model is the limit of the Gaussian theory when the Green function is approximated by the free-particle Green function. Semiclassically this is achieved neglecting all classical paths beyond the direct contribution.*

### 6.1.2 The non-isotropic Random Wave Models

The non-isotropic Random Wave Model for a wavefunction with Dirichlet or Neumann boundary conditions along an infinite straight line has the following two-point correlation function, founded by explicit ensemble average in the chapter III:

$$R_{D,N}^{RWM}(\vec{r}_1, \vec{r}_2) = \frac{1}{A} J_0 \left( k \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2} \right) \mp \frac{1}{A} J_0 \left( k \sqrt{(x_1 - x_2)^2 + (y_1 + y_2 - 2y_0)^2} \right). \quad (6.1)$$

Using the green-function approach, we consider the limiting situation when  $\vec{r}_1, \vec{r}_2$  both lie close to a boundary. Semiclassically, this means that only

the direct path joining  $\vec{r}_1$  and  $\vec{r}_2$  (which gives the isotropic contribution) and the classical trajectory starting at  $\vec{r}_1$  and ending at  $\vec{r}_2$  after one bounce contribute. The one-bounce path  $p$  is uniquely characterized by the position  $\vec{r}_p$  where it is reflected. The path length is  $L_p = L_{1p} + L_{2p}$  with  $L_{1p} = |\vec{r}_1 - \vec{r}_p|$ ,  $L_{2p} = |\vec{r}_2 - \vec{r}_p|$ . Denoting by  $\kappa_p$  and  $\theta_p$  the local boundary curvature and reflection angle after hitting the boundary and using the semiclassical formulae for the correlation function we get

$$R_{D,N}(\vec{r}_1, \vec{r}_2) \simeq \frac{1}{A} J_0(k|\vec{r}_1 - \vec{r}_2|) + \left| 2\kappa_p \left( \frac{L_{ip}L_{jp}}{L_p \cos \theta_p} \right) - 1 \right|^{-\frac{1}{2}} \times \frac{1}{A\sqrt{2\pi k L_p}} \cos \left( kL_p - \frac{\pi}{4} + \phi_p^{D,N} \right). \quad (6.2)$$

Here  $\phi_p^D = 0$  and  $\phi_p^N = \pi/2$  take into account the boundary conditions at the reflection point, as given e.g. in [75]. This expression is the exact asymptotic limit of the Random Wave Model result Eq. (6.1) in the limit of flat boundaries ( $\kappa_p \rightarrow 0$ ).

In the exact quantum mechanical description the same construction holds, but it comes from pure geometrical considerations when we apply the method of images to construct the exact Green function for the free particle in the infinite half-space. In any case, the result Eq. (6.1) is exactly recovered and we conclude that *the ensemble of random wave functions constructed to satisfy Dirichlet or Neumann boundary conditions along an infinite straight line is the limiting case of the Gaussian theory for points close to an almost straight boundary, when the semiclassical correlation function is well approximated by considering only contributions coming from the direct and one-bounce trajectories.*

In section 2.4.4 a non-isotropic Random Wave Model was presented which describes the existence of an infinite potential ramp. As usual, the statistics are Gaussian and we just need to provide a microscopic derivation of the corresponding two-point correlation function using our approach. Let us remind the result obtained by ensemble average over the assumed random superposition of basis functions:

$$R_S^r(\vec{r}_1, \vec{r}_2) = \left( \frac{2\pi^3}{\hbar^4 V} \right)^{\frac{1}{3}} \int_0^\infty \cos(Q(x_1 - x_2)) \times \text{Ai} \left[ \left( \frac{V}{\hbar^2} \right)^{\frac{1}{3}} \left( y_1 - \frac{E - \hbar^2 Q^2}{V} \right) \right] \text{Ai} \left[ \left( \frac{V}{\hbar^2} \right)^{\frac{1}{3}} \left( y_2 - \frac{E - \hbar^2 Q^2}{V} \right) \right] dQ. \quad (6.3)$$

In this case, even when explicit asymptotics can be obtained using the semiclassical Green function, it is far more illustrative to find the exact quantum mechanical Green function and use it to construct the correlation.

For a particle in the potential  $V(x, y) = Vy$ , the Schrödinger equation is separable. The solutions are plane waves along the  $x$  direction and Airy functions in the  $y$  direction,

$$\psi_{k,e}(x, y) = \left( \frac{8\pi^3}{4\hbar^4 V} \right)^{\frac{1}{6}} \exp(-ikx) \text{Ai} \left[ \left( \frac{V}{\hbar^2} \right)^{\frac{1}{3}} \left( y - \frac{e}{V} \right) \right], \quad (6.4)$$

and for the Green function

$$G(\vec{r}_1, \vec{r}_2, E + i0^+) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{\psi_{k,e}(\vec{r}_1) \psi_{k,e}^*(\vec{r}_2)}{E - e - \frac{\hbar^2 k^2}{2m} + i0^+} de dk. \quad (6.5)$$

After taking imaginary part and integrate over  $e$ , gives exactly the result of the Random Wave Model Eq. (6.3).

In the vicinity of the potential ramp only two classical trajectories join two given points for fixed energy. One path has no turning points and can be called “direct”, and the second has one turning point and is then “reflected”. Adding up this two contributions gives again the  $\hbar_{eff} \rightarrow 0$  asymptotics of the exact quantum result. *The non-isotropic RWM constructed to satisfy the Schrödinger equation in the vicinity of an infinite straight potential ramp is the limit of the Gaussian theory for points close to an almost straight smooth boundary.*

The only known example of a non-isotropic Random Wave Model describing a situation where the exact quantum mechanical Green function cannot be explicitly calculated was proposed by Berry. It is a generalization of the Random Wave Model for an infinite straight barrier, but with mixed boundary conditions,

$$\left( k\psi_M^{RWM}(\vec{r}) \cos \alpha + \frac{\partial \psi_M^{RWM}(\vec{r})}{\partial y} \sin \alpha \right) |_{y=y_0=0} = 0, \quad (6.6)$$

with  $\alpha$  a parameter interpolating between the Dirichlet ( $\alpha = 0$ ) and Neumann ( $\alpha = \pi/2$ ) cases. This example is illustrative of the power of the semiclassical approach, since the calculations are almost trivial using the semiclassical Green function. The two-point correlation function in this case was calculated by ensemble average to be,

$$R_M^r(\vec{r}_1, \vec{r}_2) = \frac{1}{2\pi A} \int_0^{2\pi} f_\alpha(y_1, \theta) f_\alpha(y_2, \theta) \cos(k(x_1 - x_2) \cos \theta) d\theta, \quad (6.7)$$

where

$$f_\alpha(y, \theta) = \frac{\cos \alpha \sin(ky \sin \theta) - \sin \alpha \sin \theta \cos(ky \sin \theta)}{\sqrt{\cos^2 \alpha + \sin^2 \alpha \sin^2 \theta}}. \quad (6.8)$$

Observe the increase in the complexity of the results compared with the Dirichlet and Neumann cases. Also, one is almost invariably interested in the asymptotics of the results when  $k \rightarrow \infty$ , and it is quite difficult to take this limit in Eq. (6.7).

Using the semiclassical method we approximate the correlation function by taking only the direct and one-bounce classical trajectories joining the points  $\vec{r}_1$  and  $\vec{r}_2$ . Applying our formulae we get exactly the same result as in the Dirichlet and Neumann cases for the correlation function,

$$R_{D,N}(\vec{r}_1, \vec{r}_2) \simeq \frac{1}{A} J_0(k|\vec{r}_1 - \vec{r}_2|) + \left| 2\kappa_p \left( \frac{L_{ip}L_{jp}}{L_p \cos \theta_p} \right) - 1 \right|^{-\frac{1}{2}} \times \frac{1}{A\sqrt{2\pi k L_p}} \cos \left( kL_p - \frac{\pi}{4} + \phi_p^\alpha \right), \quad (6.9)$$

but the extra phase is given semiclassically by  $\phi_p^\alpha = \arctan(\alpha \cos \theta_p)$ . In the limit of flat boundaries, the semiclassical result gives the correct asymptotics of the result found by Berry. The extra phase, a somehow unexpected feature in the Random Wave Model approach, finds in our semiclassical considerations its explanation in dynamical terms. *The non-isotropic RWM constructed to satisfy mixed boundary conditions along an infinite straight boundary is a Gaussian field. Its two-point correlation function is obtained by approximating the exact Green function by a sum over only direct and one-bounce classical trajectories, including a phase factor taking care of the boundary conditions at the bounce point.*

With this result, we conclude the microscopic derivation of the correlation functions for the Random Wave Models. We mention that deviations to this results has been found, particularly due to the non-zero curvature of the boundaries in realistic systems. This deviations are correctly described in our approach, where the two-point correlation function explicitly contains curvature terms.



## 6.2 Derivation of the Ballistic Sigma Model results

In this section we use the Gaussian theory supplemented with the semiclassical correlation function to find the results of the Ballistic Sigma Model. Such results emerge in the limit of infinite system's area and in situations where oscillatory contributions can be neglected. To start, a few words about the very different structure (both physical and mathematical) of the two approaches are relevant.

In the Gaussian approach, the statistical structure of the theory is assumed to be universally described by a Gaussian random field, while all the system-specific information is encoded in the fluctuations of the correlation matrix, which is finally expressed in terms of classical trajectories. On the other hand the Nonlinear Sigma Model predicts for the two-point correlation function the universal Bessel-like dependence, while the system-specific corrections appear as deviations from the Gaussian behavior of the averages, expressed finally in terms of the classical diffusive propagator.

It is not surprising then that the equivalence of the two theories at the level of the universal (Gaussian statistics and Bessel correlations) results has been established some years ago, but it has been claimed that the Gaussian theory can not incorporate effects beyond the universal limit. We will prove now that the Gaussian theory is not only able to account for the same effects beyond universality predicted by the Ballistic Sigma Model, but in fact goes beyond by incorporating correctly oscillatory contributions.

The Sigma Model results are expressed in terms of classical objects called propagators (see the appendix). To finally establish the connection with the Ballistic Sigma Model we must find the limit where our results can be expressed in terms of the classical propagator.

### 6.2.1 One point statistics

We start with the simplest statistical measure, the moments of the intensity,

$$\langle \psi(\vec{r})^{2n} \rangle = R_{2n}(\vec{r}_1 = \vec{r}, \dots, \vec{r}_n = \vec{r}). \quad (6.10)$$

We use the general formula Eq. (5.28) with  $i = j = k = o = 1$  for the non-oscillatory contribution to the averages. The universal coefficients are easily calculated using formula (5.27), since the Gaussian integrations with

$F(v) = v^{2n}$  are trivial,

$$\begin{aligned}
\mathcal{F}^{RMT} &= \langle v^{2n} \rangle_{RMT} = \frac{(2n-1)!!}{A(e)^n}, \\
\mathcal{F}^{1,1,1} &= A(e) \langle v^{2n+2} \rangle_{RMT} = \frac{(2n+1)!!}{A(e)^n}, \\
\mathcal{F}^{1,1,1,1} &= A(e)^2 \langle v^{2n+4} \rangle_{RMT} - 2A(e) \langle v^{2n+2} \rangle_{RMT} + 3 \langle v^{2n} \rangle_{RMT} \\
&= \frac{1}{A(e)^n} ((2n+3)!! - 2(2n+1)!! + 3(2n-1)!!).
\end{aligned} \tag{6.11}$$

With this partial results we can construct the universal coefficient for the non-oscillatory contribution  $F^{1,1} = A(e)^{-n} 4n(n-1)(2n-1)!!$ , and obtain finally

$$\langle \psi(\vec{r})^{2n} \rangle^{n.o} = \frac{(2n-1)!!}{A(e)^n} \left[ 1 + n(n-1) \frac{\hbar}{2\pi m^2} \sum_{\gamma} |D_{\gamma}| \Gamma^2(T_{\gamma}/\tau_W) \right], \tag{6.12}$$

where the sum extends over classical trajectories starting and ending at position  $\vec{r}$ .

Using the relationship Eq. (A.11) presented in the appendix, the sum over classical paths is related with the projection on configuration space of the classical ballistic propagator at given energy  $U_{ball}(\vec{r}, \vec{r}, t, e)$  by

$$\sum_p |D_{\gamma}| \Gamma^2(T_{\gamma}/\tau_W) = \int_0^{\infty} U_{ball}(\vec{r}, \vec{r}, t, e) \Gamma^2(t/\tau_W) dt. \tag{6.13}$$

If we now take the limit  $\delta e \rightarrow 0$ , namely  $\tau_W \rightarrow \infty$  (the meaning of which will be discussed in a moment) we get

$$\begin{aligned}
\lim_{\delta e \rightarrow 0} \langle \psi(\vec{r})^{2n} \rangle^{n.o} &= \frac{(2n-1)!!}{A(e)^n} \left[ 1 + n(n-1) \frac{\hbar}{2\pi m^2} \int_0^{\infty} U_{ball}(\vec{r}, \vec{r}, t, e) dt \right] \\
&= \frac{(2n-1)!!}{A(e)^n} [1 + n(n-1)\kappa],
\end{aligned} \tag{6.14}$$

with

$$2\pi m^2 \kappa = \hbar \Pi_{ball}(\vec{r}, \vec{r}, 0, e). \tag{6.15}$$

This is our final result. It shows that in the limit where the energy interval  $W$  is taken to be infinitely small, the non-oscillatory contributions to

the average show deviations from the Random Matrix Theory result which are proportional to the classical Green function of the Liouville equation. *Eq. (6.14) is the prediction of the Ballistic Sigma Model for  $\langle \psi(\vec{r})^{2n} \rangle$  obtained using supersymmetry methods [66].*

To proceed with less trivial examples we calculate now the full intensity distribution,

$$I(t, \vec{r}) = \langle \delta(A(e)\psi(\vec{r})^2 - t) \rangle. \quad (6.16)$$

Using the formula for the universal coefficients a straight forward calculation yields for the correction to the Random Matrix Theory result in the non-oscillatory contribution

$$\left( \frac{3}{4} - \frac{3t}{2} + \frac{t^2}{4} \right) \frac{\hbar}{2\pi m^2} \sum_{\gamma} |D_{\gamma}| \Gamma^2(T_{\gamma}/\tau_W), \quad (6.17)$$

and in the limit of a small energy window we obtain,

$$\lim_{\delta e \rightarrow 0} \langle \delta(A(e)\psi(\vec{r})^2 - t) \rangle^{n.o} = \frac{e^{\frac{t}{2}}}{\sqrt{2\pi w}} \left[ 1 + \frac{\kappa}{2} \left( \frac{3}{2} - 3t + \frac{t^2}{2} \right) \right], \quad (6.18)$$

which is the result predicted by the Ballistic Sigma Model [66].

### 6.2.2 Two point statistics

Now we turn our attention to statistical measures involving more than one position. The first non trivial example is given by the two-point correlation of the intensity,

$$R_4(\vec{r}_1, \vec{r}_1, \vec{r}_2, \vec{r}_2) = \langle \psi(\vec{r}_1)^2 \psi(\vec{r}_2)^2 \rangle. \quad (6.19)$$

In this case we have two degrees of freedom  $\vec{v} = (\psi(\vec{r}_1), \psi(\vec{r}_2))$  and  $F(\vec{v}) = v_1^2 v_2^2$ . For the non-oscillatory contribution the relevant universal coefficients are easily found with,

$$\mathcal{F}^{RMT} = \frac{1}{A(e)^2} \quad (6.20)$$

$$F^{1,1} = F^{2,2} = 0 \quad (6.21)$$

$$F^{1,2} = F^{2,1} = \frac{4}{A(e)^2}.$$

And we obtain for the non-oscillatory contribution

$$\langle \psi(\vec{r}_1)^2 \psi(\vec{r}_2)^2 \rangle^{n.o} = \frac{1}{A(e)^2} \left[ 1 + 2 \frac{\hbar}{2\pi m^2} \sum_{\gamma} |D_{\gamma}| \Gamma^2(T_{\gamma}/\tau_W) \right]. \quad (6.22)$$

In the limit of a small energy window it reads

$$\lim_{\delta e \rightarrow 0} \langle \psi(\vec{r}_1)^2 \psi(\vec{r}_2)^2 \rangle^{n.o} = \frac{1}{A(e)^2} \left[ 1 + 2 \frac{\hbar}{2\pi m^2} \Pi_{ball}(\vec{r}_1, \vec{r}_2, w=0, e) \right], \quad (6.23)$$

which is, as expected, the result found using the Ballistic Sigma Model [66].

### 6.2.3 A closer look to the disordered-ballistic transition

In the last section we have derived formal expressions for the diagonal contribution to known statistical measures using only the Gaussian conjecture and the semiclassical expression for the two-point correlation function. In order to obtain the results of the ballistic Sigma Model we made two further assumptions:

- We must neglect non-diagonal contributions, and
- We must consider the (highly pathological) limit of zero-width energy window.

We will now discuss these two extra approximations.

The non-appearance of oscillatory terms in the results of the Ballistic Sigma Model is a heritage of the same feature in its diffusive version. The oscillatory terms predicted by the semiclassical approach have typically the form

$$\langle \dots \rangle^{osc} \sim \cos \frac{S}{\hbar}. \quad (6.24)$$

What is the mechanism present in the disordered case that washes out the oscillatory contributions to the statistical measures? The answer is obvious, *in the disordered case, the extra average over position or disordered potential is the mechanism responsible for washing out the oscillatory corrections, leaving only the non-oscillatory results.* When the zero-disorder limit is taken such oscillations are not recovered, since they are not perturbative in nature,

and what is left is a theory of ballistic systems without oscillatory terms, namely, the Ballistic Sigma model.

Now let us focus on the second element in our derivation of the Ballistic Sigma Model results, the pathological limit  $\delta e \rightarrow 0$ . In our terminology this simply means the limit where the statistics reflects the behavior of a single eigenfunction. This is of course a non-analytical limit, and the fact that the Ballistic Sigma Model results need it must draw our attention to something mathematically delicate in its formulation (we remark that this limit is responsible for the strong practical limitations of the Ballistic Sigma Model. The reason is that while the semiclassical results explicitly contain a cut-off time for the period of the classical paths involved, given by the size of the energy window  $\tau_W = \hbar/\delta e$ , there is not such a scale in the Ballistic Sigma Model results and the classical propagator must be constructed for infinite time, a calculation even more difficult than solving the Schrödinger equation).

In disordered systems the limit  $\delta e \rightarrow 0$  is perfectly defined as long as the additional average over disorder provides enough eigenfunctions around a given energy to make the window size as small as one wants (this imposes certain requirements on the disorder potential). The key point is that the limits  $\delta e \rightarrow 0$  and vanishing disorder are not compatible and the ballistic limit of the Nonlinear Sigma Model demands both limits to be taken. In other words, in order to the limit of vanishing energy window to exist, we must have an ensemble of systems. *The Ballistic Sigma Model describes eigenfunctions for a given energy belonging to an ensemble of systems, while the semiclassical theory describes an ensemble of eigenfunctions around certain energy belonging to the same quantum system.* Each type of averaging introduces a time scale ( $\tau_W$  in the spectral average, and the mean free time in the disorder case) and they cannot be both taken to infinity simultaneously without making the average ill-defined.

## 6.3 A note about scars

As mentioned in the introduction, the scarring phenomena (the enhancement of the mean intensity around short periodic orbits), can not be explained on the basis of the divergent Gutzwiller Green function. A correct theory of scarring comes only when one uses a resummed version of the semiclassical Green function having the correct analytical properties.

It is then clear that the semiclassical theory presented here can not incorporate scarring effects, since we make explicit use of the Gutzwiller Green function. Once we derive the results of the Ballistic Sigma Model, it is clear also that such theory can not predict effects due to the existence of scars.

## Chapter 7

# Practical applications of the theory: tunneling rates in irregular quantum dots

In the previous chapter we have shown how to obtain all the known theories describing the statistical properties of eigenfunctions as particular limiting cases of the semiclassical. After spending some effort in this formal direction, we can now turn our attention to a more practical issue and use our theory to describe and/or understand effects experimentally measurable. We stress that by “experimental” we meant both measurements in the lab as well as exact quantum mechanical numerical calculations.

### 7.1 General considerations

Modern lithography techniques allow the construction of electronic devices where the movement of electrons is strongly localized in one direction, while in the other two directions the electron remains in a confined two-dimensional domain, the so-called 2D electron gas [76]. Such structure is called a quantum dot and we are interested in the usual experimental set-up where the number of electrons in the dot ranges from 100 to 300. When leads are attached to the dot, transport measurements can be used to probe a variety of electronic properties. In particular, for low enough temperatures and in the absence of inelastic scattering, the transport properties show strong signatures of quantum coherence [77].

In order to construct almost closed quantum dots, tunneling barriers are located between the dot and the leads. In certain regime of temperature, number of electrons and height of the tunnel barriers, the system enters in the so-called Coulomb Blockade (CB) regime where transport is strongly suppressed due to charging effects unless certain degeneracy condition is fulfilled and then the transport is dominated by resonant tunneling [77]. In the experiments, the CB effect is characterized by well defined peaks in the conductance as function of the energy, the so-called CB peaks, each corresponding to a particular resonance of the dot.

The CB conductance peak heights have been measured (see [78]), while the distribution of tunneling widths in the CB regime has been studied numerically (see [57, 79]) and used to perform numerical calculations of the conductance peaks.

Our goal in this section is to use the semiclassical approach to explicitly calculate the distribution of widths and conductances in the CB regime and compare with existing numerical and analytical results.

All the theoretical approach to the statistical characterization of the resonance widths at the level of the single particle description go in the following direction (all the symbols will be defined in a moment):

- First, a statistical distribution  $P(\psi)$  of the wavefunctions is adopted,
- such distribution is used to calculate, within a given model for the lead wavefunctions, the statistical distribution  $P(\gamma)$  of the channel decay amplitudes and,
- with this distribution (and assuming the widths corresponding to different leads to be uncorrelated) one constructs the distribution of total widths  $P(\Gamma)$ .
- Finally, the distribution of conductances  $P(g)$  can be calculated using the distribution of widths.

It is then clear that different assumptions for the distribution of wavefunction's amplitudes will correspond to different approximations for the distribution of widths. When the assumption about the wavefunctions is universal like in the Random Matrix Theory or the isotropic Random Wave Model, the results will be universal in the sense that it will only depend on the relative position and structure of the leads, not on any specific feature of the quantum



dot. On the contrary, if the distribution of wavefunctions is the one given by our approach, not only the universal but also oscillatory and non-oscillatory dot-dependent effects will be predicted.

The state of art of the problem using universal statistics for the wavefunction is given by the theory presented in [79] where Berry's ansatz was used to calculate the distribution of widths. This theory generalizes all the approaches based on the Random Matrix Theory and the isotropic Random Wave Model presented so far [80, 81], but can not be extended to dot-dependent effects. In fact, the result of a very lengthly and non trivial calculation turns out to be disappointing: the Random Wave Model predicts the same results obtained by a simple Random Matrix Theory calculation. The semiclassical approach will provide a clean explanation for this result.

The incorporation of dot-dependent effects in the theory is relevant due to the experimental observation of correlations in the CB height peaks [82], an effect beyond the universal picture. Besides the (partially phenomenological) attempts presented in [56] to incorporate scattering effects, the only explicit calculation of non-universal contributions to the distribution of widths and conductances was presented in [57]. Although this approach is in spirit similar to ours, technical problems make impossible to use it beyond the simplest case of two leads supporting one channel each. Besides, the results of [57] are strongly dependent of the particular model for the lead wavefunctions, and they completely fail to incorporate dot-dependent effects beyond the first oscillatory contribution.

We are going to follow exactly the same general approach as in the previous works, but we will not make any assumption about the lead wavefunctions, neither on the statistical independence of the different leads. We will merely follow the general approach described in the last chapter and present the results up to second semiclassical order. Our theory will be adequate to any system with any kind of boundary conditions and any number of channels and leads. We will show how to obtain the Random Matrix Theory and Random Wave Model results in the zeroth semiclassical order and we will explain the origin of the discrepancies found in previous works.

We are interested in the regime of isolated resonances where the width  $\Gamma_l$  of the dot's  $l$ -th internal single particle eigenstate and the mean level spacing  $\Delta(e_n)$  satisfy

$$\Delta(e_n) \gg \Gamma_n. \quad (7.1)$$

This condition expresses that transport is mediated by resonant tunneling

through a single internal eigenstate, say  $\psi_l(\vec{r})$ , such that its corresponding eigenenergy matches the energy of the incoming and outgoing fluxes.

## 7.2 Model and definitions

We consider an irregular quantum dot (for simplicity modeled as a billiard of area  $A$ ). The dot is weakly coupled to  $T$  leads (denoted by  $\sigma = 1, \dots, T$ ) by means of surface contacts  $\partial_\sigma$ . The leads support  $N_\sigma$  open channels, each described by the channel wavefunctions  $\phi_{e_l, \alpha_\sigma}(\vec{r})$ . Here  $\alpha_\sigma$  is an integer labeling the transversal eigenstates of the  $\sigma$ -lead while the longitudinal component of the lead wavefunction is a plane wave with wavenumber  $k_{\alpha_\sigma}$ .

The formal theory of scattering then is used to obtain the partial decay amplitude of the  $l$ -th state into the  $\alpha_\sigma$  channel of the  $\sigma$ -th lead [83]

$$\gamma_{\alpha_\sigma, l}^\sigma = \sqrt{\frac{\hbar^2 k_{\alpha_\sigma}}{m}} \int_{\partial_\sigma} \phi_{e_l, \alpha_\sigma}(\vec{r}) \psi_l(\vec{r}) d\vec{r}. \quad (7.2)$$

This relation can be used to calculate the joint distribution

$$P(\Gamma_1, \dots, \Gamma_T) = \frac{1}{N_W} \sum_{e_l \in W} \prod_{\sigma=1}^T \delta(\Gamma_\sigma - \Gamma_{l, \sigma}) \quad (7.3)$$

of the fluctuating decay widths

$$\Gamma_{l, \sigma} = \sum_{\alpha_\sigma=1}^{N_\sigma} |\gamma_{\alpha_\sigma, l}^\sigma|^2. \quad (7.4)$$

The physical origin of the correlations between the decay widths is that they are all related with the same eigenfunction inside the dot, and we have extensively shown that such object has strong spatial correlations (both universal and non-universal). In general the joint distribution of widths  $P(\Gamma_1, \dots, \Gamma_T)$  can not be factorized due to the classical trajectories starting at one lead and ending at a different one. This effect, neglected in all previous approaches, is fully taken into account in our calculation.

## 7.3 The Gaussian conjecture in action

By means of the Gaussian conjecture, we transform the spectral average Eq. (7.3) into a Gaussian integral. Following section 4.1, the calculation of

the joint distribution of widths is reduced to the calculation of the functional integral

$$P(\Gamma_1, \dots, \Gamma_T) = \int \frac{\exp \left[ \int \int \psi(\vec{r}_1) (R^{-1})(\vec{r}_1, \vec{r}_2) \psi(\vec{r}_2) d\vec{r}_1 d\vec{r}_2 \right]}{\sqrt{\det R}} \times \prod_{\sigma=1}^T \delta \left( \Gamma_{\sigma} - \left| \sqrt{\frac{\hbar^2 k_{\alpha\sigma}}{m}} \int_{\partial_{\sigma}} \phi_{e, \alpha\sigma}(\vec{r}) \psi(\vec{r}) d\vec{r} \right|^2 \right) D[\psi(\vec{r})]. \quad (7.5)$$

Here  $e$  is the energy at the center of the spectral window  $W$  (as usual the resulting distribution depends parametrically on it).  $R(\vec{r}_1, \vec{r}_2)$  is the two-point correlation function and the integral kernel  $(R^{-1})(\vec{r}_1, \vec{r}_2)$  is its functional inverse,

$$\int (R^{-1})(\vec{r}_1, \vec{r}) R(\vec{r}, \vec{r}_2) d\vec{r} = \delta(\vec{r}_1 - \vec{r}_2). \quad (7.6)$$

To start with the calculation, the Gaussian distribution is used for a finite partition of the contact surfaces and the integrals are easily calculated. After the continuous limit is recovered we obtain a closed expression for the characteristic function of the distribution  $P(\Gamma_1, \dots, \Gamma_T)$ . Introducing the vectors  $\vec{\Gamma} = (\Gamma_1, \dots, \Gamma_T)$  and  $\vec{k} = (k_1, \dots, k_T)$ , the distribution of widths is finally expressed as,

$$P(\vec{\Gamma}) = \frac{1}{(2\pi)^T} \int_{-\infty}^{\infty} \frac{e^{-i\vec{k} \cdot \vec{\Gamma}}}{\left[ \det(\mathbf{I} - 2i\mathbf{K}(\vec{k})\mathbf{G}) \right]^{1/2}} d\vec{k}, \quad (7.7)$$

where all the information about the system is encoded in the hermitian channel-channel correlation matrix  $\mathbf{G}$ . This is a  $(T \times \sum_{\sigma=1}^T N_{\sigma})$ - dimensional matrix with block structure. The (square) diagonal blocks (“reflections”) have dimension  $N_{\sigma}$  each

$$\mathbf{G}^{\sigma, \sigma} = \mathbf{r}^{\sigma}, \quad (7.8)$$

and the off-diagonal blocks (“transmissions”)

$$\mathbf{G}^{\sigma, \sigma'} = \mathbf{t}^{\sigma, \sigma'}. \quad (7.9)$$

are  $N_{\sigma} \times N_{\sigma'}$  rectangular matrices.

Each block is given in terms of the semiclassical two-point correlation function  $R$  and lead wavefunctions as

$$\begin{aligned} r_{\alpha\sigma,\beta\sigma}^\sigma &= \int_{\partial_\sigma} \int_{\partial_\sigma} \phi_{e,\alpha\sigma}(\vec{r}_1) R(\vec{r}_1, \vec{r}_2) \phi_{e,\beta\sigma}(\vec{r}_2) d\vec{r}_1 d\vec{r}_2, \\ t_{\alpha\sigma,\beta\sigma'}^{\sigma,\sigma'} &= \int_{\partial_\sigma} \int_{\partial_{\sigma'}} \phi_{e,\alpha\sigma}(\vec{r}_1) R(\vec{r}_1, \vec{r}_2) \phi_{e,\beta\sigma'}(\vec{r}_2) d\vec{r}_1 d\vec{r}_2. \end{aligned} \quad (7.10)$$

The matrices  $\mathbf{I}$  and  $\mathbf{K}(\vec{k})$  have block-diagonal structure. For  $\mathbf{I}$  each of the  $T$  blocks is the  $N_\sigma$ - dimensional unit matrix  $\mathbf{I}_\sigma$ , and for  $\mathbf{K}(\vec{k})$  each block is  $k_\sigma$  times the  $N_\sigma$ - dimensional unit matrix.

## 7.4 Separating the direct-path contribution

In order to analyze the partial result Eq. (7.7) we will separate as usual the direct-path contribution of the correlation function:

$$R(\vec{r}_1, \vec{r}_2) = \frac{1}{A} (R_0(|\vec{r}_1 - \vec{r}_2|) + \tilde{R}(\vec{r}_1, \vec{r}_2)), \quad (7.11)$$

with  $R_0(|\vec{r}_1 - \vec{r}_2|) = J_0((\sqrt{2me}/\hbar)|\vec{r}_1 - \vec{r}_2|)$  and  $\tilde{R}(\vec{r}_1, \vec{r}_2)$  given by the sum over classical paths Eq. (3.6). This separation induces a similar decomposition on the reflection and transmission blocks in the channel-channel correlation matrix. We are going to consider only the situation where there are no direct classical paths joining different leads, since this direct contribution must be calculated separately and can be avoided by placing the leads in an asymmetric configuration and/or by placing an obstacle in between.

Neglecting direct paths between leads, the entries of the reflection blocks take the form  $r_{\alpha\sigma,\beta\sigma}^\sigma = (1/A)(r_{\alpha\sigma,\beta\sigma}^{\sigma,0} + \tilde{r}_{\alpha\sigma,\beta\sigma}^\sigma)$ , and the transmission blocks are  $t_{\alpha\sigma,\beta\sigma'}^{\sigma,\sigma'} = (1/A)\tilde{t}_{\alpha\sigma,\beta\sigma'}^{\sigma,\sigma'}$  with

$$\begin{aligned} r_{\alpha\sigma,\beta\sigma}^{\sigma,0} &= \int_{\partial_\sigma} \int_{\partial_\sigma} \phi_{\alpha\sigma}(e, \vec{r}_1) J_0\left(\frac{\sqrt{2me}}{\hbar}|\vec{r}_1 - \vec{r}_2|\right) \phi_{\beta\sigma}(e, \vec{r}_2) d\vec{r}_1 d\vec{r}_2 \\ \tilde{r}_{\alpha\sigma,\beta\sigma}^\sigma &= \int_{\partial_\sigma} \int_{\partial_\sigma} \phi_{\alpha\sigma}(e, \vec{r}_1) \tilde{R}(\vec{r}_1, \vec{r}_2) \phi_{\beta\sigma}(e, \vec{r}_2) d\vec{r}_1 d\vec{r}_2, \\ \tilde{t}_{\alpha\sigma,\beta\sigma'}^{\sigma,\sigma'} &= \int_{\partial_\sigma} \int_{\partial_{\sigma'}} \phi_{\alpha\sigma}(e, \vec{r}_1) \tilde{R}(\vec{r}_1, \vec{r}_2) \phi_{\beta\sigma'}(e, \vec{r}_2) d\vec{r}_1 d\vec{r}_2. \end{aligned} \quad (7.12)$$

In the same way, the channel-channel correlation matrix is also separated as

$$\mathbf{G} = \frac{1}{A}(\mathbf{G}^0 + \tilde{\mathbf{G}}), \quad (7.13)$$

and the matrix in the denominator of Eq. (7.7) defining the joint distribution of widths can be written as,

$$\mathbf{I} - 2i\mathbf{K}(\vec{k})\mathbf{G} = (\mathbf{I} - 2i\mathbf{K}(\vec{k})\mathbf{G}^0) \left[ \mathbf{I} - 2i \frac{2i\mathbf{K}(\vec{k})\tilde{\mathbf{G}}}{\mathbf{I} - 2i\mathbf{K}(\vec{k})\mathbf{G}^0} \right]. \quad (7.14)$$

We observe now that by construction the matrix  $\mathbf{I} - 2i\mathbf{K}(\vec{k})\mathbf{G}^0$  is block-diagonal and its determinant is just the product of the determinants of its diagonal blocks. Using this fact we can finally write the joint distribution of widths as

$$P(\vec{\Gamma}) = \frac{1}{(2\pi)^T} \int_{-\infty}^{\infty} \left[ \prod_{\sigma=1}^T \frac{e^{-ik_{\sigma}\Gamma_{\sigma}}}{\sqrt{\det(\mathbf{I}_{\sigma} - 2ik_{\sigma}A^{-1}\mathbf{r}^{\sigma,0})}} \right] \times \quad (7.15)$$

$$\left[ \det \left( \mathbf{I} - 2i \frac{2i\mathbf{K}(\vec{k})\tilde{\mathbf{G}}}{\mathbf{I} - 2i\mathbf{K}(\vec{k})\mathbf{G}^0} \right) \right]^{-1/2} d\vec{k},$$

which is as far as we can go using only the Gaussian conjecture for eigenfunctions. Eq. (7.15) is the starting point to derive all previous results and to provide general expressions in the semiclassical regime.

The distribution of widths Eq. (7.15) depends on particular details of the system under study due to the following effects:

- position and structure of the leads and,
- the specific shape of the dot.

The separation  $\mathbf{G} = (1/A)(\mathbf{G}^0 + \tilde{\mathbf{G}})$  allows to distinguish clearly between the two sources of deviations from universality: all the information about the leads is encoded into the direct part of the reflection matrices  $\mathbf{r}^{\sigma,0}$ , while the shape of the dot is encoded in the non-direct part of both the reflection and transmission matrices  $\tilde{\mathbf{r}}^{\sigma}, \tilde{\mathbf{t}}^{\sigma}$ . We will explore the kind of results obtained by neglecting one or both sources of system-specific effects.

## 7.5 Derivation of the Random Matrix Theory and Random Wave Model results

The first and crudest approximation we can consider is to neglect all dot-specific effects, namely

$$\tilde{\mathbf{G}}^{RMT} = 0, \quad (7.16)$$

and to consider the reflection matrices as proportional to the unity matrix on each subspace (they cannot be taken as zero since their diagonal elements are positive definite),

$$\tilde{\mathbf{r}}^{\sigma,0,RMT} = A^{-1} \bar{\Gamma}^\sigma \mathbf{I}_\sigma. \quad (7.17)$$

Under this approximations, the distribution of widths takes the form

$$\begin{aligned} P^{RMT}(\vec{\Gamma}) &= \frac{1}{(2\pi)^T} \int_{-\infty}^{\infty} \left[ \prod_{\sigma=1}^T \frac{e^{-ik_\sigma \Gamma_\sigma}}{(1 - 2ik_\sigma \bar{\Gamma}_\sigma)^{N_\sigma/2}} \right] d\vec{k} \\ &= \prod_{\sigma=1}^{N_\sigma} \left[ \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{e^{-ik \Gamma_\sigma}}{(1 - 2ik \bar{\Gamma}_\sigma)^{N_\sigma/2}} \right] \end{aligned} \quad (7.18)$$

$$= \prod_{\sigma=1}^{N_\sigma} P_\sigma^{RMT}(\Gamma_\sigma), \quad (7.19)$$

as the product of the RMT width distribution for each lead, easily calculated using residues to be the celebrated  $\chi^2$ -distribution [84],

$$P_\sigma^{RMT}(\Gamma_\sigma) = \frac{\Gamma_\sigma^{N_\sigma/2-1} e^{-\Gamma_\sigma/2\bar{\Gamma}_\sigma}}{(2\bar{\Gamma}_\sigma^2)^{N_\sigma/2} (N_\sigma/2 - 1)!}. \quad (7.20)$$

This result is the fully universal limit of the theory, independent of any system parameter besides the average widths  $\bar{\Gamma}_\sigma$  and the number of channels in each lead  $N_\sigma$ . It has been derived using a variety of methods [79–81].

The next step towards the incorporation of system-specific effects was taken independently by Efetov and Iia (using supersymmetry methods [80]), and Alhassid and Lewenkopf (using the isotropic Random Wave Model [79]). It consists, finally, in including the effects of the particular configurations of the leads and lead wavefunctions, while keeping the Random Matrix Theory model for the dot. For historical reasons (it was believed that the calculation went beyond the Random Matrix Theory for the dot's description, which is not the case) we call this approximation the Random Wave Model result.

In the framework of our general expression, The system-specific effects due to the leads are included by taking

$$\tilde{\mathbf{G}}^{RWM} = 0, \quad (7.21)$$

and the reflection matrices being non-diagonal. The results are complicated expressions in terms of the eigenvalues of the reflection matrices, but the joint distribution still factorizes

$$P^{RWM}(\vec{\Gamma}, \mathbf{G}^0) = \prod_{\sigma=1}^{N_\sigma} P_\sigma^{RWM}(\Gamma_\sigma, \mathbf{r}^{\sigma,0}). \quad (7.22)$$

Different choices for the lead wavefunctions will produce different matrices  $\mathbf{r}^{\sigma,0}$  and then different results. However, it can be shown [85] that *if the leads are modeled as hard walls waveguides, the direct-path reflection matrices  $\mathbf{r}^{\sigma,0}$  are strictly diagonal, i.e. the Random Wave Model and Random Matrix Theory results will be identical.* This simple observation explains why the results in [79] obtained by using the isotropic Random Wave Model but *hard-wall waveguides* gave no deviations from the Random Matrix Theory predictions.

It is clear that the kind of non-universal effects we want to investigate, the ones due only to the particular classical dynamics inside the dot, are fully contained in the non-direct part of the channel-channel correlation matrix. This effects are much more difficult to analyze due to the structure of the resulting integral, which in particular do not factorize. The analysis of this very interesting regime is the subject of the next section.

## 7.6 Beyond the Random Matrix Theory: The full semiclassical program

So far we have used only the Gaussian conjecture for the dot's eigenfunctions. Now, we the expression Eq. (7.7), we can pursue the second part of the semiclassical program: expanding the expressions up to second semiclassical order.

In this case we must expand the integrand in Eq. (7.7) up to second order in the components of the matrix  $\tilde{\mathbf{G}}$ . We note also that the  $k$ -integrations are taken along the real line, and since the integrand is perfectly well behaved

for real  $k$  due to the positiveness and symmetry of the matrix  $\mathbf{r}^0$ , we can expand the determinant and calculate the integrals to obtain the analog of the general result Eq. (8.1) in the space of channels:

$$\begin{aligned}
P(\vec{\Gamma}) = P^{RMM}(\vec{\Gamma}, \mathbf{G}_0) &+ \sum_{\sigma}^T \sum_{\alpha_{\sigma}, \beta_{\sigma}}^{N_{\sigma}} P^{\alpha_{\sigma}, \beta_{\sigma}}(\vec{\Gamma}, \mathbf{G}_0) \tilde{r}_{\alpha_{\sigma}, \beta_{\sigma}}^{\sigma} \\
&+ \sum_{\sigma}^T \sum_{\alpha_{\sigma}, \beta_{\sigma}, \gamma_{\sigma}, \eta_{\sigma}}^{N_{\sigma}} P^{\alpha_{\sigma}, \beta_{\sigma}, \gamma_{\sigma}, \eta_{\sigma}}(\vec{\Gamma}, \mathbf{G}_0) \tilde{r}_{\alpha_{\sigma}, \beta_{\sigma}}^{\sigma} \tilde{r}_{\gamma_{\sigma}, \eta_{\sigma}}^{\sigma} \\
&+ \sum_{\sigma, \sigma'}^T \sum_{\alpha_{\sigma}, \beta_{\sigma}, \gamma_{\sigma'}, \eta_{\sigma'}}^{N_{\sigma}, N_{\sigma'}} P^{\alpha_{\sigma}, \beta_{\sigma}, \gamma_{\sigma'}, \eta_{\sigma'}}(\vec{\Gamma}, \mathbf{G}_0) \tilde{t}_{\alpha_{\sigma}, \beta_{\sigma}}^{\sigma} \tilde{t}_{\gamma_{\sigma'}, \eta_{\sigma'}}^{\sigma'}.
\end{aligned} \tag{7.23}$$

The universal coefficients  $P^{RMM}(\vec{\Gamma}, \mathbf{G}_0)$ ,  $P^{\alpha_{\sigma}, \beta_{\sigma}, \gamma_{\sigma}, \eta_{\sigma}}(\vec{\Gamma}, \mathbf{G}_0)$ ,  $P^{\alpha_{\sigma}, \beta_{\sigma}, \gamma_{\sigma'}, \eta_{\sigma'}}(\vec{\Gamma}, \mathbf{G}_0)$  have closed expressions depending only on the number and structure of the leads and they are fully independent on the dynamics inside the dot. In this sense they are universal.

The general formula for the distribution of widths Eq. (7.23) implies two important predictions:

- The first system-specific contribution to the Random Wave Model results is oscillatory. It is expressed as a sum over classical trajectories starting and ending at the same lead at given initial and final channel and it is not present in the Ballistic Sigma Model results, obtained by taking only non-oscillatory contributions.
- Besides the non-oscillatory contributions to the second semiclassical order, there are contributions from nonlinear mixing of channels (the non-diagonal terms in the double sums).

Now we will discuss the relevance of this results to describe experimental and/or numerical data.

## 7.7 Relevance for numerical and experimental results

Once the distribution of widths is obtained, it can be used to calculate observable quantities. In particular, the conductance measured between two leads



(say  $\sigma = 1$  and  $\sigma = 2$ ) in the CB conductance peak corresponding to the  $l$ -th resonance, is given by [86]

$$g_{1,2}^{(l)} = \frac{e^2}{h} \frac{\pi}{2k_B T} \frac{\Gamma_{l,1} \Gamma_{l,2}}{\Gamma_{l,1} + \Gamma_{l,2}}, \quad (7.24)$$

and we are interested in its statistical fluctuations when the energy (or  $l$ ) is varied.

The distribution of conductances  $P_g(g_{1,2})$  is explicitly written in terms of the distribution of widths as

$$P_g(g_{1,2}) = \int_0^\infty \delta \left( g_{1,2} - \frac{e^2}{h} \frac{\pi}{2k_B T} \frac{\Gamma_1 \Gamma_2}{\Gamma_1 + \Gamma_2} \right) P(\Gamma_1, \Gamma_2) d\Gamma_1 d\Gamma_2, \quad (7.25)$$

and the general structure of the distribution of widths Eq. (7.23) leads to a similar structure for the distribution of conductances,

$$\begin{aligned} P_g(g_{1,2}) = & P_g^{RMM}(g_{1,2}, \mathbf{G}_0) + \sum_{\sigma=1,2} \sum_{\alpha_\sigma, \beta_\sigma}^{N_\sigma} P_g^{\alpha_\sigma, \beta_\sigma}(g_{1,2}, \mathbf{G}_0) \tilde{r}_{\alpha_\sigma, \beta_\sigma}^\sigma \\ & + \sum_{\sigma=1,2} \sum_{\alpha_\sigma, \beta_\sigma, \gamma_\sigma, \eta_\sigma}^{N_\sigma} P_g^{\alpha_\sigma, \beta_\sigma, \gamma_\sigma, \eta_\sigma}(g_{1,2}, \mathbf{G}_0) \tilde{r}_{\alpha_\sigma, \beta_\sigma}^\sigma \tilde{r}_{\gamma_\sigma, \eta_\sigma}^\sigma \\ & + \sum_{\alpha_1, \beta_1, \gamma_2, \eta_2}^{N_1, N_2} P_g^{\alpha_1, \beta_1, \gamma_2, \eta_2}(g_{1,2}, \mathbf{G}_0) \tilde{t}_{\alpha_1, \beta_1}^{1,2} \tilde{t}_{\gamma_2, \eta_2}^{2,1}. \end{aligned} \quad (7.26)$$

This our final (and fully general) result for the distribution of conductances. All results previously reported can be derived as limiting cases of this formula. The universal coefficients in this case are complicated functions of the conductance  $g_{1,2}$  and the eigenvalues of the matrix  $\mathbf{G}^0$ , but in any case they are independent of the dynamics inside the dot. The dot-specific contributions appear through the non-universal transmission and reflection matrices  $\tilde{\mathbf{r}}^1, \tilde{\mathbf{r}}^2, \tilde{\mathbf{t}}^{1,2}$ . The transmission and reflection matrices are expressed in terms of classical trajectories which spend a finite amount of time inside the dot and are sensitive to the dot's particular geometry.

In order to focus on the effects predicted in the semiclassical approach and to compare with previous works, we will study now the simplest possible case: two leads ( $T = 2$ ) denoted by left ( $l$ ) and right ( $r$ ), each supporting only one open channel ( $N_1 = N_2 = 1$ ), and assuming the dot to be described as a billiard system.

All the blocks of the  $\mathbf{G}$  matrix are  $1 \times 1$  (just numbers), and then the channel indexes are not necessary. The distribution of conductances  $g_{l,r} = g$  reads

$$\begin{aligned} P(g) = P^{RMM}(g, \mathbf{G}_0) &+ \sum_{i=l,r} P^i(g, \mathbf{G}_0) \tilde{r}^i \\ &+ \sum_{i=l,r} P^i(g, \mathbf{G}_0) (\tilde{r}^i)^2 \\ &+ P^{l,r}(g, \mathbf{G}_0) (\tilde{t}^{l,r})^2. \end{aligned} \quad (7.27)$$

After calculating the integrals defining the reflection and transmission numbers  $\tilde{r}^l, \tilde{r}^r$  in terms of classical trajectories, they have the following structure

$$\tilde{r}^i = \sum_{\gamma_i} A_{\gamma_i} \cos \left( \frac{i}{\hbar} S_{\gamma_i} \right), \quad i = l, r \quad (7.28)$$

as sums over classical paths  $\gamma_i$  starting and ending in the same lead  $i$ , where  $A_{\gamma_i}$  are smooth functions of the energy and  $S_{\gamma_i}$  the classical action. For the transmissions we have in analogy,

$$\tilde{t}^{l,r} = \sum_{\gamma_{l,r}} A_{l,r} \cos \left( \frac{i}{\hbar} \tilde{S}_{l,r} \right), \quad (7.29)$$

in terms of classical paths starting at one lead and ending at the other.

In the case of billiard systems, the actions of the classical paths are given by  $S_\gamma = \hbar k L_\gamma$  with  $k = \sqrt{2me}/\hbar$  the wavenumber corresponding to the energy at the center of the spectral window, and  $L_\gamma$  the length of the path. Now we can easily see the main predictions of our results.

First, *the distribution of conductances as a function of the energy (or wavenumber) at the center of the spectral window presents modulations on top of the Random Matrix Results.* The modulations in energy of the CB conductance distribution appear in both leading and sub-leading semiclassical order. According to our results, in leading order the frequencies of the modulations are simply given by the lengths of the classical paths  $L_{\gamma_l}, L_{\gamma_r}$  starting and ending at the same lead. The second order contribution to the modulations presents non-linear mixing of the harmonics coming from different trajectories, and then frequencies like  $L_{\gamma_l} \pm L_{\gamma'_l}$  will be visible in the Fourier spectra.

The second effect predicted by our analysis is that *classical trajectories joining two different leads produce contribution of second semiclassical order, while the leading order is dominated by trajectories starting and ending at the same lead*. This is in some sense expected, since we expect the conductance to be directly related with the local density of states at the surface between lead and dot, and this in turn depends on classical trajectories starting and ending at the same point.

We want to stress that exactly the effects qualitatively predicted by our results have been observed both in experiments [82] and numerical simulations [57]. In particular, the non-linear mixing of frequencies in the CB mean conductance as function of the energy has not been explained so far. We believe our results show the origin of such effects.

To conclude, we mention that the modulations of the CB conductance statistics, as a typical oscillatory effect, is washed out when we perform an extra average, and cannot be predicted by the Ballistic Sigma Model.

The calculation of the distribution of widths and conductances in terms of universal coefficients and sums over classical trajectories shows all the features of our approach. It is based on, and only on, the Gaussian conjecture for the eigenfunctions inside the dot and a consistent semiclassical expansion of the results. It is easy to implement and its predictions agree with the available experimental and numerical data.

## Chapter 8

# Conclusions and open questions

In this thesis we have explored in detail a statistical theory of eigenfunctions in clean classically chaotic quantum systems. Our approach has two ingredients, both of them well known:

- A conjecture about the statistical behavior of irregular eigenfunctions, and
- an approximation method for the spatial two-point correlation function.

The statistical conjecture is that *in classically chaotic quantum systems, eigenfunctions belonging to a small energy window behave as realizations of a Gaussian random field*, while the approximation method is the *semiclassical approximation to the Green function as a sum over classical trajectories*.

The first part of the work was dedicated to study separately this two ingredients. From our observations we conclude:

- Although there is no formal proof of its validity, the Gaussian conjecture captures many important ingredients of what we expect the exact distributions must look like. In particular, our numerical calculations based on exact quantum mechanical data from [63] are described by the Gaussian conjecture with an impressive degree of accuracy.
- The semiclassical approximation to the two-point correlation function describes very well our numerical calculations. The agreement is by far superior compared with other existing approaches.

After testing the two ingredients of the theory, we focused on the formal implications of the resulting hybrid approach, in particular its relation to

the Random Wave Models and the Nonlinear Sigma Model, the other two standard methods to describe irregular eigenfunctions. Our results formally establish for the first time the following equivalences:

- All Random Wave Models presented so far are limiting cases of the Gaussian-semiclassical approach. They can be obtained by keeping the Gaussian conjecture, but using a microscopic two-point correlation function adapted to the particular geometry described by each particular Random Wave Model. Deviations due to the non-trivial geometry of any realistic confinement are missing in the Random Wave Model descriptions, but are correctly incorporated in the semiclassical approach.
- The Ballistic Sigma Model is a limiting case of the Gaussian-semiclassical theory where oscillatory contributions to the results are systematically neglected and the energy window is made arbitrarily small. The Ballistic Sigma Model is missing oscillatory contributions to the results which are correctly incorporated by the semiclassical approach.

This two facts allow us to conclude that, to date, the theory presented here is the most general approach for the statistical description of irregular eigenfunctions in clean systems.

Finally, we have presented a practical application of the methods in the realm of quantum interference effects in mesoscopic devices. Using our ideas we have calculated the distribution of tunneling widths in an almost closed quantum dot in the Coulomb Blockade regime. Our results are the most general ones presented so far since they rely only on the Gaussian conjecture and the well-controlled semiclassical approximation. This allows for a detailed comparison with previous works to conclude that:

- Deviations from universality in the statistics of tunneling widths and conductances are due to two separate mechanisms, the structure and position of the leads and the dynamics inside the dot.
- The deviations due to the system-specific classical dynamics inside the dot produce oscillations on top of the universal results when the energy window is moved along the spectrum. The leading oscillatory effects come from classical trajectories entering into the dot with given energy, channel, and lead and returning to the same lead. The sub-leading semiclassical order is given in terms of pairs of trajectories starting and

ending at the same lead, and pairs of trajectories joining two different leads

The available results of both numerical and experimental works support our conclusions.

Our fundamental result, encoding the Gaussian conjecture and the consistent treatment of the semiclassical approximation, is the general expression Eq. (8.1) for an arbitrary statistical measure  $\mathcal{F}$ ,

$$\begin{aligned}\mathcal{F} = \mathcal{F}^{RMT} &+ \frac{1}{2} \sum_{i,j}^n \mathcal{F}^{i,j} \tilde{R}_{i,j} - \frac{1}{2} \sum_{i,j,k}^n \mathcal{F}^{i,j,k} \tilde{R}_{i,k} \tilde{R}_{k,j} \\ &+ \frac{1}{8} \sum_{i,j,k,o}^n \mathcal{F}^{i,j,k,o} \tilde{R}_{i,j} \tilde{R}_{k,o},\end{aligned}$$

which is the most general structure of any average calculated in the framework of the Gaussian-semiclassical approach. It expresses the statistical measure  $\mathcal{F}$  in terms of universal functions  $\mathcal{F}^{i,\dots}$  that are independent of the particular system, and sums over system-specific classical trajectories (encoded in  $\tilde{R}_{i,j}$ ). Although such general expression has not been derived using any other approach, Eq. (8.1) contains as particular cases all results coming from the Random Wave Models, the Ballistic Sigma Model and the Nonlinear Sigma Model (in the non-localized regime).

Putting all the pieces together, we conclude that **all the available numerical, experimental, and theoretical evidence supports the idea that for statistics involving a set of points of zero measure, the probability distribution of eigenfunctions is indeed Gaussian**. This remark shows the importance of understanding the microscopic origin of this behavior, a task that our work puts at the level of the most fundamental open problem in the field of irregular eigenfunctions.

# Appendix A

## The classical diffusive and ballistic propagators

Semiclassical methods are based on the construction of quantum mechanical quantities using classical ones. In the Gutzwiller formulation of the semiclassical Green function, the classical objects involved are the classical trajectories and classical periodic orbits, while in the Nonlinear Sigma Model and its ballistic counterpart, the Ballistic Sigma Model, the quantum mechanical results are approximated by expressions involving another kind of classical objects called propagators. In this appendix we formally define such objects, introduce some notations frequently used in our work and present related classical objects called probabilities of propagation.

Consider a partial differential equation of the form

$$\mathcal{L}(x, \partial_x)f(x, t) = \frac{\partial f(x, t)}{\partial t} \quad (\text{A.1})$$

for a suitable well behaved pseudo-differential operator  $\mathcal{L}$ , hermitian under some scalar product in a space of smooth enough functions  $f$ . Since Eq. (A.1) is a first-order equation in the time, its solution is given by

$$f(x, t) = \int U_{\mathcal{L}}(x, x', t)f(x', 0)dx', \quad \text{for } t > 0, \quad (\text{A.2})$$

which defines the time-dependent propagator, or simply *propagator*,  $U_{\mathcal{L}}(x, x', t)$ . Using Dirac notation, we write  $f(x, t) = \langle x|f(t)\rangle$  and the propagator is formally expressed as

$$U_{\mathcal{L}}(x, x', t) = \langle x|e^{\mathcal{L}t}|x'\rangle. \quad (\text{A.3})$$

The associate Green function, or *frequency-dependent propagator*, is its Laplace transform,

$$\Pi_{\mathcal{L}}(x, x', w) = \int_0^\infty e^{-iwt} U_{\mathcal{L}}(x, x', t) dt, \quad (\text{A.4})$$

and it is formally expressed as

$$\Pi_{\mathcal{L}}(x, x', w) = \left\langle x \left| \frac{1}{iw - \mathcal{L}} \right| x' \right\rangle. \quad (\text{A.5})$$

If the solutions of the equation A.1 are positive defined and normalized over  $x$  for all times, they admit a probabilistic interpretation, and the time dependent propagator is then interpreted as the probability to find a particle at point  $x$  in time  $t$  if it was at point  $x'$  in time  $t = 0$ . In particular, the quantity

$$\begin{aligned} P_{\mathcal{L}}(x, x') &:= \int_0^\infty U_{\mathcal{L}}(x, x', t) dt \\ &= \Pi_{\mathcal{L}}(x, x', 0) \end{aligned} \quad (\text{A.6})$$

has the interpretation of a *total probability of propagation from  $x$  to  $x'$* . In the case of  $x=x'$ ,  $P_{\mathcal{L}}(x, x')$  is known as the total probability of return.

In the diffusive case, the phase space is just the configuration space  $x := \vec{r}$ , the functions are densities defined on it and normalized under the usual  $L_2$  norm and the pseudo differential operator is the diffusion operator,

$$\mathcal{L}_{diff} = -D\nabla^2 \quad (\text{A.7})$$

with suitable boundary conditions.  $\langle \vec{r}_i | e^{\mathcal{L}_{diff}t} | \vec{r}_f \rangle$  is then called diffusive propagator  $U_{diff}$ . The diffusive Green function, total probability of diffusive propagation and total probability of diffusive return follow immediately.

In the ballistic case, the phase space is the symplectic manifold of Hamiltonian dynamics, with local coordinates given by position and momentum  $x := (\vec{r}, \vec{p})$ , the functions are densities defined on it specifying the probability to find a particle at a given point in phase space, while the scalar product is the usual  $L_2$  norm with the Liouville measure  $dx = d\vec{r}d\vec{p}$ . The pseudo differential operator is the Liouville operator (Poisson bracket)

$$\mathcal{L}_{ball} = \frac{\partial H}{\partial \vec{r}} \cdot \frac{\partial}{\partial \vec{p}} - \frac{\partial H}{\partial \vec{p}} \cdot \frac{\partial}{\partial \vec{r}} \quad (\text{A.8})$$



with suitable boundary conditions.  $\langle \vec{r}_i | e^{\mathcal{L}_{ball}t} | \vec{r}_f \rangle$  is called ballistic (or Frobenius-Perron) propagator  $U_{ball}$ . All the other quantities follow directly.

Since the Hamiltonian dynamics takes place, in the conservative case, along manifolds of constant energy in phase space and the results of this thesis are almost always referred to configuration space, we define the projection onto configuration space at constant energy of the ballistic probability of propagation as

$$U_{ball}(\vec{r}_i, \vec{r}_f, t, e) = \int \delta(e - H(\vec{r}_i, \vec{p}_i)) U_{ball}(\vec{r}_i, \vec{p}_i, \vec{r}_f, \vec{p}_f, t) d\vec{p}_i d\vec{p}_f, \quad (\text{A.9})$$

which induces a similar projection for the ballistic Green function

$$\Pi_{ball}(\vec{r}_i, \vec{r}_f, w, e) = \int \delta(e - H(\vec{r}_i, \vec{p}_i)) \Pi_{ball}(\vec{r}_i, \vec{p}_i, \vec{r}_f, \vec{p}_f, w) d\vec{p}_i d\vec{p}_f, \quad (\text{A.10})$$

and a similar interpretation for  $\Pi_{ball}(\vec{r}_i, \vec{r}_f, w = 0, e) = \int_0^\infty U_{ball}(\vec{r}_i, \vec{r}_f, t, e) dt$  as the total probability of ballistic propagation from position  $\vec{r}_i$  to position  $\vec{r}_f$  at given energy  $e$ . A fundamental result widely used in this work is the fact that  $U_{ball}(\vec{r}_i, \vec{r}_f, t, e)$  can be calculated in terms of the classical paths joining  $\vec{r}_i$  and  $\vec{r}_f$  for given time  $t$  and energy  $e$ . The result is [53]

$$U_{ball}(\vec{r}_i, \vec{r}_f, t, e) = \sum_{\gamma} |D_{\gamma}(\vec{r}_i, \vec{r}_f)| \delta(t - T_{\gamma}), \quad (\text{A.11})$$

which establishes the link between the semiclassical approximation, given in terms of the amplitudes  $\sqrt{|D_{\gamma}(\vec{r}_i, \vec{r}_f)|}$ , and the Frobenius-Perron propagator.

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# Acknowledgments

Taking a look over the last four years, some things appear now with great clarity, and some lessons are here with me to stay. I want to thank Klaus for showing an almost infinite degree of patience with me and a good deal of faith in my work and ideas. Little by little, and sometimes without my own conviction, he has taught me how the best way to respect our work as scientists is to present our ideas standing over the firm ground of our results, and how this does not mean that our imagination cannot fly. This is a basic principle of the ethical exercise of science I learnt from him, and it will stay with me.

The Graduiertenkolleg "Nichtlinearität und Nichtgleichgewicht in kondensierter Materie" has been a solid financial help, and I am glad I can retribute some of this help with my work. The basic philosophy and motivations of the Kollegue gave me the chance to interact with people for other scientific communities, something that has enriched my research.

My all-life friends have been there in the good and in the bad times. It has been an honour and a pleasure for me to move through the years together with Carlos, Ricardo, Guillermo, Clara, Adriana and Javier. It is also a pleasure to share with them the passion for a good book, a nice movie and a perfect song.

My Mother Fe, my father Fernando, my brother Luis Fernando and my sister Martha Liliana have been always in my heart. They will be forever a reference point in my life, showing me that, at the end, love and understanding are good reasons to keep on trying to be better persons.

The semiclassics-mesoscopic-molecular-cold atoms-gang at the institut of physics in Regensburg has given me the change to meet fantastic people, with whom I hope I will stay in contact. Marko, the "loop guy" always gave a very objective and usefull comment about my problems, both related and non related with physics. Peter has showed me his very personal way to deal with life, and introduced me to many books, music, movies and ideas I will keep with me. Andy was able to be my office partner for two years without getting crazy, something to admire indeed. Jörg showed me how to be a professional of the semiclassical methods and an ethernal admirer of beauty. Niels has walked with me the travel of perceptions, and he has never failed. I spent a great time with all of you, thanks.

Katalin has given me the strenght to go on and fight for my ideas and dreams. There are no words to express how important she has been for me, and what an honour for me is to have her in my arms.

Juan Diego.